

Validation documentation
APIs & excipients, solid

HiperScan GmbH

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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, solid*.

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

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

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

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

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

Criteria for the inclusion of substances

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

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

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

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

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

Validation concept

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

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

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

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

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

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

Model creation procedure and validation runs

The safety of the [chemometric models](#) is guaranteed by several measures during model creation, of which the validation step is the final one. Normally, the procedure is as follows. It is in particular valid for the active pharmaceutical ingredients (APIs) *solid API excipients*, *liquid/semi-solid API excipients (with a test certificate)*, *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 generated. These also include spectra from substances which the *chemometric model* should not identify, but were also recorded during generation in order to increase selectivity. (As a result, the model “learns” to differentiate from other substances which are actually unknown to it.)
- b) *Type B*: Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database. These also include reference spectra of other substance classes, and spectra that are not used as reference spectra. Samples are considered to be independent, if they originate from a batch, of which no spectra have been used for the generation of the database. (Up to *IdentModule 2018-01*, samples were still considered independent if the sampling was done independently, i.e. if they originate from another sales container.)
- c) *Type C*: Spectra from the field, which have not been recorded under the control of *HiperScan GmbH* and have not been used for the generation of the database. The spectra include not only substances of the substance class to be tested, but also substances from other classes.

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

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

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

4. Validation runs and approval

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

Particularities of individual substance classes

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

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

Also, for the substance class **PhytoComm** (TCM-Granulated herbal extracts of the manufacturer *PhytoComm*) spectra for all useable batches are recorded by *HiperScan GmbH* and entered in the database. The supplier organises the respective tests themselves and keeps the test certificates.

A new evaluation option was created for the class *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 the supplier *PhytoComm*, whereby all useable batches from the supplier are known.

The *PhytoComm* class can only confirm the identity of batches that have been used for the generation of the database. As a consequence there cannot be any validation spectra of other batches. Therefore, the criterion reads that two samples (from different sales containers) from each batch must exist, one for the structure of the database (*Type A*) and one for the validation (*Type B*).

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 database *PhytoComm* 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, em Huang Qi granulate from the company *PhytoComm* neither needs to be delimited from *Huang Qi* granulate from the company *HerbaSinica* 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 $\mathbf{X}$.

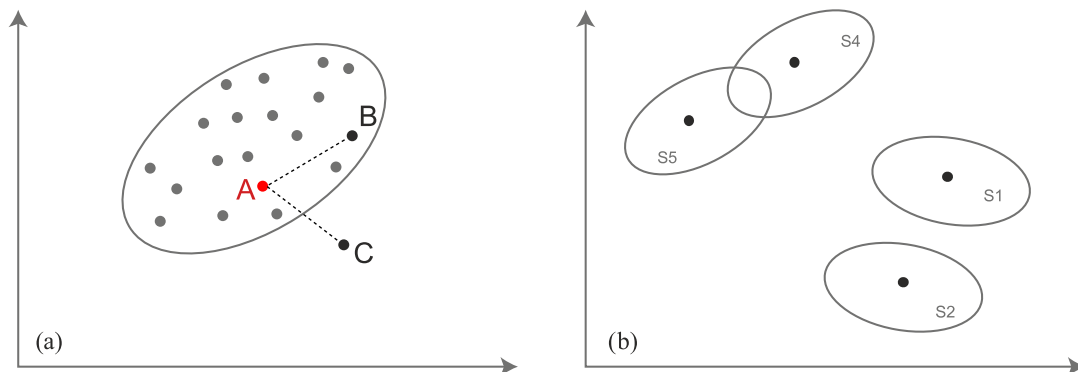


Figure 1: (a) The *Mahalanobis distance* from *A* to *B* is less than from *A* to *C*. However, the *Euclidean distances* are identical. (b) The *Mahalanobis distance* between the two measurement series *S4* and *S5* is smaller than between *S1* and *S2*. However, the *Euclidean distances* are identical.

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].

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

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

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

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

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

Summary

A total of 280 317 spectra from 29 123 different batches for a total of 847 substances were used to validate the substance class *APIs & excipients, solid*.

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, solid	344	1529	68 246
Specific classifier 26188	9	17	720
Narcotic substances, solid	15	71	5230
Drugs	5	6	300

From category *A* a total of 74 496 spectra from 1623 batches for a total of 373 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, solid	490	2171	98 590
Drugs	265	502	23 103
Narcotic substances, solid	17	98	4530
Specific classifier 26188	10	18	669

From category *B* a total of 126 892 spectra from 2789 batches for a total of 782 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, solid	396	20 482	64 723
Drugs	284	5714	13 411
Narcotic substances, solid	13	384	794
Specific classifier 26188	1	1	1

From category *C* a total of 78 929 spectra from 26 581 batches for a total of 694 substances were taken into account for validation.

Validation results

The validation runs checked whether all substances/substance groups in the substance class *APIs & excipients, solid* 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, solid* 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	68 034	132	23 770 554
Type B	0	85 138	3147	40 516 668
Type C	0	59 846	3114	25 194 287

All substances/substance groups in the substance class *APIs & excipients, solid* 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 96 %)	99.802 60 % (> 99.796 80 %)
Type B	100.000 00 % (> 99.999 97 %)	95.996 62 % (> 95.991 09 %)
Type C	100.000 00 % (> 99.999 63 %)	91.409 76 % (> 91.322 88 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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 2.0-2019-02

Validated substance/substance group **Acetylcysteine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20040-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Acetylcysteine; Acetylcysteinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Acetylcysteine*:

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

Validation samples

A total of 280 317 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 *Acetylcysteine*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 6 reference samples from the substance/substance group *Acetylcysteine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Acetylcysteine	1208026-01	21628 [†]	20
Euro OTC	Acetylcysteine	1510016	22228 [†]	20
Caelo	Acetylcysteine	161398	22469 [†]	20
Caelo	Acetylcysteine	163340	23035	40
Euro OTC	Acetylcysteine	1801037	23956	40
Euro OTC	Acetylcysteine	1809026	24302	40

- 126 712 spectra from a total of 2783 batches from further 781 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*.

- 23 spectra from 19 *Apo-Ident* customers from 20 batches from the substance/substance group *Acetylcysteine*.

Supplier	Substance	Batch	Spectra
Caelo	Acetylcysteine	12299004	1
Fagron	Acetylcysteine	13A22N07	1
Caelo	Acetylcysteine	10230713	1
Caelo	Acetylcysteine	12299021	1
Euro OTC	Acetylcysteine	12299010	1
Euro OTC	Acetylcysteine	120802601	2
Caelo	Acetylcysteine	12299027	1
Caelo	Acetylcysteine	130702601	1
Phönix	Acetylcysteine	1208026	1
Phoenix goettin	Acetylcysteine	1208026-01	1
Caelo	Acetylcysteine	15114007	1
Caelo	Acetylcysteine	15114013	2
Caelo	Acetylcysteine	16139802	1
Sanacorp 07.03.2016 10,...	Acetylcysteine	15114007	1
Euro OTC	Acetylcysteine	1510016-01	1
Caelo	Acetylcysteine	16139808	1
Euro OTC	Acetylcysteine	1505011-01	1
Gehe	Acetylcysteine	16139813	1
Caelo	Acetylcysteine	1011171701	1
Farmalabor	Acetylcysteine	P1701913-003	1
Caelo	Acetylcysteine	16334006	1

- 78 906 spectra from 565 *Apo-Ident* customers from a total of 26 117 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Acetylcysteine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Acetylcysteine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	180	0	126 712
Type C	0	23	0	78 906

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 73.9130 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21315	22469	8.62	83.83
21628	22469	3.21	80.04
22228	22228	0.00	81.07
22469	22469	0.00	79.14
22886	22469	9.10	82.67
22854	22854	0.00	83.19

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Acetylsalicylic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20449-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Acetylsalicylic acid; Acidum acetylsalicylicum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Acetylsalicylic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetylsalicylic ...	13297509	21383	40	20131014
Euro OTC	Acetylsalicylic ...	1307024-01	21597	30	20130904
Euro OTC	Acetylsalicylic ...	1407026-01	21637	40	20140801
Euro OTC	Acetylsalicylic ...	1601042	22377	40	20160204*
Euro OTC	Acetylsalicylic ...	1608037	22820	40	20160921*
Caelo	Acetylsalicylic ...	161316	23064	40	20160825*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 230 spectra of 6 reference samples from the substance/substance group *Acetylsalicylic acid*. These samples are listed above in the [calibration samples](#) section.
- 74266 spectra from a total of 1617 batches from further 372 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 [†].

- 235 spectra of 7 reference samples from the substance/substance group *Acetylsalicylic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Acetylsalicylic acid	1307024-01	21597 [†]	15
Euro OTC	Acetylsalicylic acid	1407026-01	21637 [†]	20
Fagron	Acetylsalicylic acid	14E02-B04-297099	22949	40
Euro OTC	Acetylsalicylic acid	1703010	23388	40
Caelo	Acetylsalicylic acid	173098	23806	40
Euro OTC	Acetylsalicylic acid	1805004	24120	40
Euro OTC	Acetylsalicylic acid	1805003	24127	40

- 126657 spectra from a total of 2782 batches from further 781 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*.

- 122 spectra from 77 *Apo-Ident* customers from 56 batches from the substance/substance group *Acetylsalicylic acid*.

Supplier	Substance	Batch	Spectra
Euro OTC	Acetylsalicylic acid	1011015-01	1
Gehe	Acetylsalicylic acid	10365302	1
Caelo	Acetylsalicylic acid	10099907	1
Euro OTC	Acetylsalicylic acid	20030611-1	1
Euro OTC	Acetylsalicylic acid	1107007-01	1
Caelo	Acetylsalicylic acid	12212219	1
Noweda	Acetylsalicylic acid	10040403	1
Caelo	Acetylsalicylic acid	11257126	1
Caelo	Acetylsalicylic acid	12212203	1
Caelo	Acetylsalicylic acid	12212223	3
Euro OTC	Acetylsalicylic acid	1212005-01	3
Caelo	Acetylsalicylic acid	12212230	1
Caelo	Acetylsalicylic acid	12212236	2
Caelo	Acetylsalicylic acid	12212233	1
Caelo	Acetylsalicylic acid	12212234	2
Euro OTC	Acetylsalicylic acid	1307024-01	6
Bombastus	Acetylsalicylic acid	1212005-01	1
Caelo	Acetylsalicylic acid	13324101	1
Sanacorp	Acetylsalicylic acid	1307024-01	1
Caelo	Acetylsalicylic acid	13324109	3
Sanacorp	Acetylsalicylic acid	13324109	1
Caelo	Acetylsalicylic acid	13324119	1
EuRho	Acetylsalicylic acid	1307024-01	2
Caelo	Acetylsalicylic acid	13297511	1
Phoenix	Acetylsalicylic acid	13324107	1
Phönix	Acetylsalicylic acid	13324114	1
Caelo	Acetylsalicylic acid	13324118	1
Euro OTC	Acetylsalicylic acid	1407025-01	16
Euro OTC	Acetylsalicylic acid	1407025	1
Caelo	Acetylsalicylic acid	13324105	1
Caelo	Acetylsalicylic acid	14189603	1
Caelo	Acetylsalicylic acid	14250101	1
sanacorp	Acetylsalicylic acid	14250101	1
EuRo Gehe	Acetylsalicylic acid	147026-01	1
Caelo	Acetylsalicylic acid	13324116	1
Caelo	Acetylsalicylic acid	15081301	3
ACM	Acetylsalicylic acid	KNC2077J14	1
ACM	Acetylsalicylic acid	KNC2152J13	1
Euro OTC	Acetylsalicylic acid	1501046-01	4
Caelo	Acetylsalicylic acid	301115	1
Caelo	Acetylsalicylic acid	15081308	2
Caelo	Acetylsalicylic acid	15122701	1
Caelo	Acetylsalicylic acid	15081304	1
Caelo	Acetylsalicylic acid	15334902	2
Caelo	Acetylsalicylic acid	15334907	4
Caelo	Acetylsalicylic acid	15334910	1
Euro OTC	Acetylsalicylic acid	815A-01012	1
Caesar & Loretz GmbH	Acetylsalicylic acid	15334914	1
Caelo	Acetylsalicylic acid	15334914	3
Caelo	Acetylsalicylic acid	15081310	1
Caelo	Acetylsalicylic acid	17023102	6
Caelo	Acetylsalicylic acid	15334917	1
Caelo	Acetylsalicylic acid	1110417	1
Caesar & Loretz GmbH	Acetylsalicylic acid	15334917	1
Caelo	Acetylsalicylic acid	16131607	2

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Supplier	Substance	Batch	Spectra
Caelo	Acetylsalicylic acid	17023108	2
Caelo	Acetylsalicylic acid	17023107	7
Caelo	Acetylsalicylic acid	1061117/17023107	1
Caelo	Acetylsalicylic acid	17023111	1
Caelo	Acetylsalicylic acid	17023110	5
Phoenix/Cealo	Acetylsalicylic acid	17356301	1
Caelo	Acetylsalicylic acid	17329204	1
Sanacorp	Acetylsalicylic acid	17329204	1
Caelo	Acetylsalicylic acid	18122602	1

- 78 807 spectra from 565 *Apo-Ident* customers from a total of 26 082 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Acetylsalicylic 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 *Acetylsalicylic 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	230	0	74 266
Type B	0	235	0	126 657
Type C	0	120	2	78 807

The substance/substance group *Acetylsalicylic 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 % (> 99.9887 %)	100.0000 % (> 97.3913 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.4468 %)
Type C	100.0000 % (> 99.8817 %)	98.3607 % (> 95.9016 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21383	22377	4.68	57.41
21597	22377	6.80	56.75
21637	22820	11.82	55.78
22377	22377	0.00	56.57
22820	22820	0.00	56.52
23064	23064	0.00	57.43

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Aciclovir**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21677-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Aciclovir; Aciclovirum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Aciclovir*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Aciclovir	13B04-B40-294559	21677	40	AR-15-FG-002570-01
Fagron	Aciclovir	13B04-B40-302333	21761	40	20131217
Fagron	Aciclovir	14G07-B05-296462	21831	40	20140728

Validation samples

A total of 280 317 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 *Aciclovir*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 5 reference samples from the substance/substance group *Aciclovir*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Aciclovir	13B04-B40-294559	21677 [†]	20
Fagron	Aciclovir	13B04-B40-302333	21761 [†]	20
Fagron	Aciclovir	14G07-B05-296462	21831 [†]	20
Fagron	Aciclovir	15A15-B10-323362	22938	40
Fagron	Aciclovir	15A15-B10-323362	22939	40

- 126 752 spectra from a total of 2785 batches from further 781 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.

- 17 spectra from 8 *Apo-Ident* customers from 5 batches from the substance/substance group *Aciclovir*.

[†]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
Fagron	Aciclovir	15AS15-B10-307743	1
Fagron	Aciclovir	15A15-B10-315379	13
Fagron	Aciclovir	14g07-b05-296462	1
Fagron	Aciclovir	16K09-B05-328196	1
Fagron	Aciclovir	17G11-B01-339460	1

- 78 912 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Aciclovir* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Aciclovir* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	140	0	126 752
Type C	0	17	0	78 912

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.8817 %)	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
21677	21677	0.00	77.46
21761	21677	5.61	78.66
21831	21677	13.68	80.66

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Aescin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20377-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Aescin; Aescinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Aescin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Aescin	12K22-N13	21237	30	20121127
Euro OTC	Aescin	1310020-01	21238	20	AR-15-FG-005777-01
Euro OTC	Aescin	1506038	21838	40	20150708*
Fagron	Aescin	12I07-B40-306607	22610	40	1610369
Euro OTC	Aescin	1605021	22684	40	20160609*
Euro OTC	Aescin	1612012	22988	40	20170213*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 210 spectra of 6 reference samples from the substance/substance group *Aescin*. These samples are listed above in the [calibration samples](#) section.
- 74 286 spectra from a total of 1617 batches from further 372 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 4 reference samples from the substance/substance group *Aescin*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Aescin	12K22-N13	21237 [†]	10
Euro OTC	Aescin	1310020-01	21238 [†]	20
Euro OTC	Aescin	1506038	21838 [†]	20
Euro OTC	Aescin	1807015-01	24187	40

- 126 802 spectra from a total of 2785 batches from further 781 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*.

- 5 spectra from 2 *Apo-Ident* customers from 4 batches from the substance/substance group *Aescin*.

Supplier	Substance	Batch	Spectra
Euro OTC	Aescin	1108038	1
Euro OTC	Aescin	1310020-01	1
Fagron	Aescin	30691/M3	1
Euro OTC	Aescin	1612012-01	2

- 78 924 spectra from 565 *Apo-Ident* customers from a total of 26 133 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Aescin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Aescin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 286
Type B	0	90	0	126 802
Type C	0	3	2	78 924

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.1429 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.8819 %)	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
21237	22610	8.01	21.05
21238	21238	0.00	14.62
22610	22610	0.00	18.15
22988	22988	0.00	17.42
21838	21838	0.00	12.83
22684	22684	0.00	11.73

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Albendazole**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21596-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Albendazole; Albendazolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Albendazole*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Albendazole	12J25-B40-293217	21596	30	AR-15-FG-002571-01
Fagron	Albendazole	14B05-B41-299704	21730	40	20140430
Fagron	Albendazole	16B04-B06-322057	22968	40	20160302

Validation samples

A total of 280 317 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 *Albendazole*. These samples are listed above in the [calibration samples](#) section.
- 74 386 spectra from a total of 1620 batches from further 372 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 [†].

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

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Albendazole	12J25-B40-293217	21596 [†]	15
Fagron	Albendazole	14B05-B41-299704	21730 [†]	20
Fagron	Albendazole	14B05-B41-314321	22940	40
Fagron	Albendazole	16B04-B06-329519	23017	40

- 126 777 spectra from a total of 2785 batches from further 781 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 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Albendazole*.

Supplier	Substance	Batch	Spectra
Fagron	Albendazole	14B05B41-312959	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	Albendazole	14B05-B41	1
Fagron	Albendazole	14B05-B41-305249	1
Fagron	Albendazole	14b05-b41-314321	1
Fagron	Albendazole	14B05-B41-314321	1

- 78 924 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Albendazole* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Albendazole* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 386
Type B	0	115	0	126 777
Type C	0	5	0	78 924

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 94.5455 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.7826 %)
Type C	100.0000 % (> 99.8819 %)	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
21596	21596	0.00	73.98
21730	21596	19.89	77.55
22968	21596	18.70	76.01

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Alfatradiol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20292-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Alfatradiol; Alfatradiolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Alfatradiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Alfatradiol	13G19-N06	20940	40	1402683
Caelo	Alfatradiol	13201601	21476	80	20130812
Euro OTC	Alfatradiol	1404001-01	21714	40	1509288
Euro OTC	Alfatradiol	1603019	22511	40	20160419*
Fagron	Alfatradiol	15J27-B08-323877	22934	40	20151117

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Alfatradiol	1404001-01	21714SI	40	1509288
Euro OTC	Alfatradiol	1603019	22511SI	40	20160419*
Fagron	Alfatradiol	15J27-B08-323877	22934SI	40	20151117

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 8 reference samples from the substance/substance group *Alfatradiol*. These samples are listed above in the [calibration samples](#) section.
- 74 136 spectra from a total of 1618 batches from further 372 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 [†].

- 430 spectra of 11 reference samples from the substance/substance group *Alfatradiol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Alfatradiol	13201601	21476 [†]	40
Caelo	Alfatradiol	13201601	21477	60
Euro OTC	Alfatradiol	1404001-01	21714 [†]	10
Fagron	Alfatradiol	15J27-B08-323877	22933	40
Audor Pharma	Alfatradiol	AP33-16-I-62P2985A	22935	40
Caelo	Alfatradiol	161804	23354	40
Caelo	Alfatradiol	13201601	21477SI	60
Euro OTC	Alfatradiol	1404001-01	21714SI [†]	20
Fagron	Alfatradiol	15J27-B08-323877	22933SI	40
Audor Pharma	Alfatradiol	AP33-16-I-62P2985A	22935SI	40
Caelo	Alfatradiol	161804	23354SI	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*.

- 126 462 spectra from a total of 2784 batches from further 781 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.

- 282 spectra from 141 *Apo-Ident* customers from 114 batches from the substance/substance group *Alfatradiol*.

Supplier	Substance	Batch	Spectra
Fagron	Alfatradiol	11G22-N11	2
Fagron	Alfatradiol	11K25-N01	3
Fagron	Alfatradiol	11D07-N19	1
Caelo	Alfatradiol	11061001	2
Caelo	Alfatradiol	11161805	4
Fagron	Alfatradiol	12D19-N03	6
Caelo	Alfatradiol	11061004	1
Caelo	Alfatradiol	11061005	1
Caelo	Alfatradiol	10319909	1
Caelo	Alfatradiol	12164201	3
Fagron	Alfatradiol	11B07-N05	1
Caelo	Alfatradiol	12H29-N05	2
Fagron	Alfatradiol	12H29-N05	4
Audor Pharma	Alfatradiol	APXP103DAA	2
Caelo	Alfatradiol	11161807	3
Fagron	Alfatradiol	XP101UT	1
Hirsch	Alfatradiol	12L19-N08	2
Caesar/Lorenz	Alfatradiol	11061001	1
Fagron	Alfatradiol	12L19-N08	7
Caelo	Alfatradiol	10319904	1
Fagron	Alfatradiol	12L19-No8	1
Caelo	Alfatradiol	12164207	6
Caelo	Alfatradiol	111161607	1
Fagron	Alfatradiol	13G19-N06	19
Caesar&Loretz GmbH/Anzag	Alfatradiol	12164207	1
Audor Pharma	Alfatradiol	APXPC0071A	2
Fagron	Alfatradiol	13G19-No6	2
Fagron	Alfatradiol	11k25-N01	1
carlo	Alfatradiol	10319903	1
Caelo	Alfatradiol	13130806	2
Caelo	Alfatradiol	13130805	5
Caelo	Alfatradiol	511211	1
Fagron	Alfatradiol	13G19-N06	1
Euro OTC	Alfatradiol	121696	1
Caelo	Alfatradiol	13130808	1
Phönix	Alfatradiol	APXPC0071A	1
Fagron	Alfatradiol	13G19-N09	1
Caelo	Alfatradiol	5051406	1
Sanacorp	Alfatradiol	13201605	1
Fagron	Alfatradiol	13201605	1
Fagron	Alfatradiol	13201605	1
Fagron	Alfatradiol	13L30-B32	2
Caelo	Alfatradiol	13201605	2
VDL 1.7.14;40.30 euro	Alfatradiol	13G19-N06	1
Caelo	Alfatradiol	14037904	3

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Supplier	Substance	Batch	Spectra
Fagron	Alfatradiol	13L30B32	1
Fagron	Alfatradiol	13L30B32-290741	1
Audor Pharma	Alfatradiol	AP5100461A	2
Caelo	Alfatradiol	14139103	6
Fagron	Alfatradiol	14G07-B99-294945	4
Fagron	Alfatradiol	14C20-B02-294943	2
Caelo	Alfatradiol	14C20-B02-294943	2
Fagron	Alfatradiol	13L30-B32-290739	1
Fagron	Alfatradiol	14G07-B99-294942	1
Fagron	Alfatradiol	14G07-B99	1
Caelo	Alfatradiol	14139104	12
Fagron	Alfatradiol	13130b32290742	1
Audor Pharma	Alfatradiol	AP1404001-01A	1
Caelo	Alfatradiol	14C20-B02-294944	1
Fagron	Alfatradiol	14722-B30-302018	1
Caelo	Alfatradiol	2061504	1
Fagron	Alfatradiol	5102432	1
Fagron	Alfatradiol	14C20-B02-294944	1
Caelo	Alfatradiol	14I22-B30-302019	1
Audor Pharma	Alfatradiol	AP5104925A	6
Caelo	Alfatradiol	14139102	2
Fagron	Alfatradiol	15G07-B01-310227	4
Audor Pharma	Alfatradiol	AP1504015-01A	2
Fagron	Alfatradiol	15G07-B01-310228	3
Caelo	Alfatradiol	14130104	1
Kwizda	Alfatradiol	529068	1
Fagron	Alfatradiol	15G07-B01-310229	2
Shandong northwest manu...	Alfatradiol	AEC151211	1
Caelo	Alfatradiol	15380001	7
Fagron	Alfatradiol	12J27-B08-314546	1
Caelo	Alfatradiol	14318502	1
Caelo	Alfatradiol	15356801	15
Caelo	Alfatradiol	15G07-B01-310227	1
Fagron	Alfatradiol	15G07-B01-311881	1
Caelo	Alfatradiol	5107516	1
Fagron	Alfatradiol	15J27-B08	1
Caelo	Alfatradiol	15G07-B01-311881	1
Shandong Northwest Manu...	Alfatradiol	AEC160522	1
Phönix	Alfatradiol	15356801	1
Audor Pharma	Alfatradiol	AP514925A	1
Caelo	Alfatradiol	14139105	2
Audor Pharma	Alfatradiol	AP33-16-I-42P2945A	2
Euro OTC	Alfatradiol	1404001-01	1
Fagron	Alfatradiol	15J27-B08-318783	1
Fagron	Alfatradiol	14/22-B30-302017	1
Fagron	Alfatradiol	15J27-B08-321786	1
Caelo	Alfatradiol	1536801	1
Fagron	Alfatradiol	15G07-B01	1
Fagron	Alfatradiol	16g05-b01-324614	1
Anzag / Gehe	Alfatradiol	14C20-B02-294943	1
Sanacorp, 39,57EUR, 27.1.17	Alfatradiol	700670-0011	1
Caelo	Alfatradiol	15356804	5
Fagron	Alfatradiol	324614	1
Audor Pharma	Alfatradiol	33-16-I-62P2985A	1
Gehe	Alfatradiol	16087501	1
Fagron	Alfatradiol	15J27B08318164	1
Fagron	Alfatradiol	16G05-B01-328254	1
Audor Pharma	Alfatradiol	AP3316I62P2985A	1
Caelo	Alfatradiol	16087501	4
Fagron	Alfatradiol	16G05-B01-326866	1

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Supplier	Substance	Batch	Spectra
Audor Pharma	Alfatradiol	AP33-16-I-62P2985A	2
Fagron	Alfatradiol	16G05-B01-324614	1
Sanacorp	Alfatradiol	15356804	1
Fagron	Alfatradiol	15J27-B08-318164	3
Caelo	Alfatradiol	14318512	3
Caesar&Lorenz/Phoenix	Alfatradiol	16087502	1
Caelo	Alfatradiol	16087502	4
Fargon/Kehr	Alfatradiol	16G05-B01-332379	1
Noweda	Alfatradiol	16G05-B01-324614	1
Fagron	Alfatradiol	16G05-B01-332379	1
Caesar und Loretz GmbH	Alfatradiol	16087502	1
Fagron	Alfatradiol	16G05-B01-335789	3
Caelo	Alfatradiol	16087507	1
Caelo	Alfatradiol	16G05-B01-335789	1
Fagron	Alfatradiol	16G05-B01-325108	1
Fgron / Alliance Healthc.	Alfatradiol	16G05-B01-328254	1
Caelo	Alfatradiol	16087504	4
Audor Pharma	Alfatradiol	AP21-16-II-14P4511A	4
Fagron	Alfatradiol	16G05-B01-332379	1
Fagron	Alfatradiol	16G05-B01-334055	1
Fagron	Alfatradiol	17G03-B11	2
Fagron	Alfatradiol	16G05-801	1
Fagron	Alfatradiol	17G03-B11-345093	2
Caelo	Alfatradiol	17G03-B11-341398	1
Euro OTC	Alfatradiol	1404001-02	1
Fagron	Alfatradiol	17G03-B11-341398	1
Caelo	Alfatradiol	16087512	2
Caelo	Alfatradiol	160875105728	1
Fagron	Alfatradiol	17G03-B11-346962	1
Fagron	Alfatradiol	9011904	1
Fagron	Alfatradiol	18C23-B05-354802	1
Fagron	Alfatradiol	18C23-B05-352724	1

- 78 647 spectra from 565 *Apo-Ident* customers from a total of 26 023 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	360	0	74 136
Type B	0	430	0	126 462
Type C	0	270	12	78 647

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.6047 %)
Type C	100.0000 % (> 99.8817 %)	95.7447 % (> 94.6809 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22934	22511	2.03	24.50
22511	22511	0.00	24.37
20940	20940	0.00	24.02
21476	22511	5.28	24.32
21714	21714	0.00	19.84

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Allantoin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20079-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Allantoin; Allantoinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Allantoin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Allantoin	13I03-B05	21216	40	20130927
Euro OTC	Allantoin	1406011-01	21625	40	20140718
Euro OTC	Allantoin	1609012	22750	40	20161006*
Euro OTC	Allantoin	1609012-01	22810	40	20161006

Validation samples

A total of 280317 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 *Allantoin*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 [†].

- 260 spectra of 7 reference samples from the substance/substance group *Allantoin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Allantoin	1406011-01	21625 [†]	20
Caelo	Allantoin	162289	22756	40
Caelo	Allantoin	172346	23629	40
Caelo	Allantoin	172346	23635	40
Euro OTC	Allantoin	1406011-04	24095	40
Caelo	Allantoin	181586	24235	40
Euro OTC	Allantoin	1811006	24344	40

- 126632 spectra from a total of 2783 batches from further 781 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*.

- 284 spectra from 114 *Apo-Ident* customers from 79 batches from the substance/substance group *Allantoin*.

Supplier	Substance	Batch	Spectra
Caelo	Allantoin	11247504	5
Caelo	Allantoin	20071202	1
Fagron	Allantoin	12C30-N04	1
Caelo	Allantoin	81542358	2
Caelo	Allantoin	11247510	2
Caelo	Allantoin	140512	1
Caelo	Allantoin	20140612-15	1
Caelo	Allantoin	11247511	2
Caelo	Allantoin	12251502	2
Caelo	Allantoin	12251501	4
Sanacorp	Allantoin	12251501	1
Caelo	Allantoin	12251505	7
Caelo	Allantoin	1225101	1
Caelo	Allantoin	2713431	1
Caesar & Loretz GmbH	Allantoin	12251505	1
Caelo	Allantoin	1113E-01087	1
Fagron	Allantoin	11J11-N11	3
Caelo	Allantoin	10318313	1
Caelo	Allantoin	12251510	9
Fagron	Allantoin	13A21-N07	3
DSM Nutritional Prod./ ...	Allantoin	12251505	1
Caesar & Loretz GmbH	Allantoin	12251510	1
Caelo	Allantoin	10064015	1
Sanacorp	Allantoin	12251510	1
Caelo	Allantoin	12374401	1
Caelo	Allantoin	12251511	1
Gehe	Allantoin	12251510	1
Fagron	Allantoin	12B09-N09	1
Caelo	Allantoin	10318305	1
Caesar & Loretz GmbH	Allantoin	12374403	1
Caelo	Allantoin	10064012	1
Caelo	Allantoin	10064008	4
Caelo	Allantoin	12374403	8
Caelo	Allantoin	2264594	1
celo/Jenne	Allantoin	12374403	1
Caelo	Allantoin	12374404	2
Sanacorp	Allantoin	12374409	2
Caelo	Allantoin	12374409	15
Fagron	Allantoin	13G16-N07	6
Caelo	Allantoin	2713448	1
Caelo	Allantoin	12374407	4
Caesar & Loretz GmbH	Allantoin	12374409	1
Fagron	Allantoin	13I03-B05-289430	1
Fargron/AHD	Allantoin	13G16-N07	1
Caelo	Allantoin	5051402	1
Caelo	Allantoin	12374414	8
Caelo	Allantoin	12374415	10
Caelo	Allantoin	12374408	1
Caelo	Allantoin	10318312	1
Euro OTC	Allantoin	1401046-01	3
Phoenix 08.10.14	Allantoin	1401046-01	1
VDL 17.10.14	Allantoin	12374415	1
Fagron	Allantoin	5011E-01087	1
Euro OTC	Allantoin	1406011-01	7
Caelo	Allantoin	12374422	8

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Supplier	Substance	Batch	Spectra
Euro OTC	Allantoin	140104601	1
Anzag;18.03.15;2,76EUR	Allantoin	14247602	1
Caesar & Loretz GmbH	Allantoin	12374415	1
Caelo	Allantoin	12374417	1
Caelo	Allantoin	12374423	2
Caelo	Allantoin	14247602	6
Sanacorp	Allantoin	12374422	1
Gehe	Allantoin	14247603	1
Caesar & Loretz GmbH	Allantoin	14247602	1
Caelo	Allantoin	12374418	2
Caelo	Allantoin	14247609	7
Caelo	Allantoin	15220006	13
Caesar & Loretz GmbH	Allantoin	12374416	1
Caelo	Allantoin	15220004	1
Caelo	Allantoin	15220005	2
Euro OTC	Allantoin	1406011-02	1
Caelo	Allantoin	1522008	1
Caelo	Allantoin	4247602	1
Caelo	Allantoin	15220008	7
Euro OTC	Allantoin	140601103	1
Caelo	Allantoin	15220007	4
Caelo	Allantoin	15275302	1
Caesar&Loretz GmbH	Allantoin	12374409	1
Caelo	Allantoin	15220010	2
Caelo	Allantoin	15220012	10
Caelo	Allantoin	15220011	2
Euro OTC	Allantoin	15220008	2
Caelo	Allantoin	152200012	1
EuRho / Phoenix	Allantoin	1406011-03	1
Caelo	Allantoin	15275305	2
Caelo	Allantoin	15275312	6
Euro OTC	Allantoin	1609012-01	5
Caelo	Allantoin	16228903	8
Caelo	Allantoin	15275304	2
AHD	Allantoin	1609012-01	1
Euro OTC	Allantoin	1406011	1
Kehr	Allantoin	15220008	1
Caelo	Allantoin	28101702	1
Caelo	Allantoin	16228906	9
Caelo	Allantoin	121127	1
Caelo	Allantoin	16228904	1
Euro OTC	Allantoin	1406011-04	1
Caelo	Allantoin	16228915	14
Noweda	Allantoin	16228915	1
EuRho	Allantoin	1406011-04	1
Ichthyol-Gesellschaft	Allantoin	16228915	1
Caelo	Allantoin	17355903	1
Caelo	Allantoin	1406011-05	1
Euro OTC	Allantoin	1406011-05	1

- 78 645 spectra from 565 *Apo-Ident* customers from a total of 26 058 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Allantoin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Allantoin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	260	0	126 632
Type C	0	278	6	78 645

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.8817 %)	97.8873 % (> 96.8310 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21216	22750	5.79	37.56
21625	22750	6.50	37.49
22750	22750	0.00	38.15
22810	22750	3.19	38.78

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Allopurinol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22243-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Allopurinol; Allopurinolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Allopurinol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Allopurinol	14E15-B05-307746	22243	40	AR-16-FG-004367-01
Fagron	Allopurinol	14E15-B05-315557	22345	40	20140611

Validation samples

A total of 280 317 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 *Allopurinol*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Allopurinol*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Allopurinol	14E15-B05-307746	22243 [†]	20
Fagron	Allopurinol	14E15-B05-315557	22345 [†]	20
Fagron	Allopurinol	14E15-B05-307746	22836	40
Fagron	Allopurinol	14E15-B05-330859	23523	40
Fagron	Allopurinol	14E15-B05-330859	23526	40

- 126 732 spectra from a total of 2786 batches from further 781 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 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Allopurinol*.

[†]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
Fagron	Allopurinol	14E15-B05-315557	13
Fagron	Allopurinol	14E15-B08	1
Fagron	Allopurinol	14E15-B05-320787	1

- 78 914 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Allopurinol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Allopurinol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	160	0	126 732
Type C	0	15	0	78 914

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	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
22243	22243	0.00	87.62
22345	22243	1.16	86.52

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **alpha-tocopheryl acetate dry concentrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20433-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

alpha-tocopheryl acetate dry concentrate; alpha-Tocopherolum aceticum siccatum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *alpha-tocopheryl acetate dry concentrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	alpha-tocopheryl...	1110021-02	20907	40	20120104
Fagron	alpha-tocopheryl...	13H30-B02-287169	21609	40	AR-15-FG-006388-01
Euro OTC	alpha-tocopheryl...	1305032-01	21680	40	AR-15-FG-001194-01
Euro OTC	alpha-tocopheryl...	1507001	21842	40	20130708*
Fagron	alpha-tocopheryl...	14B03-B04-295113	21959	40	20140224
Euro OTC	alpha-tocopheryl...	1603046	22543	40	20160429*

Validation samples

A total of 280 317 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 *alpha-tocopheryl acetate dry concentrate*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 7 reference samples from the substance/substance group *alpha-tocopheryl acetate dry concentrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	alpha-tocopheryl acetate dry...	13H30-B02-287169	21609 [†]	20
Euro OTC	alpha-tocopheryl acetate dry...	1305032-01	21680 [†]	20
Euro OTC	alpha-tocopheryl acetate dry...	1507001	21842 [†]	20
Fagron	alpha-tocopheryl acetate dry...	14B03-B04-295113	21959 [†]	20
Fagron	alpha-tocopheryl acetate dry...	16H30-B05-326792	22948	40
Euro OTC	alpha-tocopheryl acetate dry...	1705003	23424	40
Euro OTC	alpha-tocopheryl acetate dry...	1810024	24309	40

- 126 692 spectra from a total of 2782 batches from further 781 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.

- 12 spectra from 8 *Apo-Ident* customers from 8 batches from the substance/substance group *alpha-tocopheryl acetate dry concentrate*.

Supplier	Substance	Batch	Spectra
Euro OTC	alpha-tocopheryl acetate dry...	1110021-02	2
Fagron	alpha-tocopheryl acetate dry...	13H30-B02-287169	1
Euro OTC	alpha-tocopheryl acetate dry...	1507001-01	2
Bombastus	alpha-tocopheryl acetate dry...	1507001-02	1
Euro/Sanacorp	alpha-tocopheryl acetate dry...	150700101	1
Kehr	alpha-tocopheryl acetate dry...	1705003-03	2
Caelo	alpha-tocopheryl acetate dry...	1705003-01	1
Sanacorp	alpha-tocopheryl acetate dry...	1705003-03	1
Euro OTC	alpha-tocopheryl acetate dry...	1705003-04	1

- 78 917 spectra from 565 *Apo-Ident* customers from a total of 26 129 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *alpha-tocopheryl acetate dry concentrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *alpha-tocopheryl acetate dry concentrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	187	13	126 692
Type C	0	11	1	78 917

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	93.5000 % (> 92.0000 %)
Type C	100.0000 % (> 99.9818 %)	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
21609	21609	0.00	43.91
21680	21680	0.00	40.88
21842	21842	0.00	43.85
22543	22543	0.00	43.60
21959	21680	5.61	40.76
20907	21680	4.36	40.71

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Ambroxol hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20742-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ambroxol hydrochloride; Ambroxoli hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Ambroxol hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ambroxol hydroch...	11110008-01	20742	40	1401146
Fagron	Ambroxol hydroch...	13I24-N02	21230	40	20131017
Euro OTC	Ambroxol hydroch...	1311032-01	21244	40	20131219
Euro OTC	Ambroxol hydroch...	1509032	21942	40	20151027*
Euro OTC	Ambroxol hydroch...	1601008	22298	40	20160119*
Euro OTC	Ambroxol hydroch...	1602015	22347	40	20160217*
Euro OTC	Ambroxol hydroch...	1604035	22550	40	20160428*

Validation samples

A total of 280 317 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 *Ambroxol hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 216 spectra from a total of 1616 batches from further 372 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 11 reference samples from the substance/substance group *Ambroxol hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ambroxol hydrochloride	1509032	21942 [†]	20
Euro OTC	Ambroxol hydrochloride	1601008	22298 [†]	20
Euro OTC	Ambroxol hydrochloride	1602015	22347 [†]	20
Caelo	Ambroxol hydrochloride	161996	22636	40
Euro OTC	Ambroxol hydrochloride	1609002	22800	40
Euro OTC	Ambroxol hydrochloride	1702004	23155	40
Caelo	Ambroxol hydrochloride	171582	23344	40
Caelo	Ambroxol hydrochloride	172860	23801	40
Euro OTC	Ambroxol hydrochloride	1711021	23894	40
Euro OTC	Ambroxol hydrochloride	1806009	24155	40
Euro OTC	Ambroxol hydrochloride	1811039	24423	40

- 126 512 spectra from a total of 2778 batches from further 781 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.

- 96 spectra from 53 *Apo-Ident* customers from 38 batches from the substance/substance group *Ambroxol hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	Ambroxol hydrochloride	12K12-N02	1
Chem & Pharma	Ambroxol hydrochloride	AXL0361201310	1
Euro OTC	Ambroxol hydrochloride	1311032-01	1
Euro/Noweda	Ambroxol hydrochloride	1509032-01	1
EuroTOC	Ambroxol hydrochloride	1602015-01	1
EuRho	Ambroxol hydrochloride	1602015-02	2
Caelo	Ambroxol hydrochloride	1602015-02	1
Phoenix	Ambroxol hydrochloride	1604035-02	1
Euro OTC	Ambroxol hydrochloride	1604035-02	5
Euro OTC	Ambroxol hydrochloride	1604035-01	1
Euro OTC	Ambroxol hydrochloride	1602015-02	1
Anzag	Ambroxol hydrochloride	15G15-B01-316109	1
Euro OTC	Ambroxol hydrochloride	ax10492201608	1
Euro OTC	Ambroxol hydrochloride	1609002-01	6
Fagron	Ambroxol hydrochloride	1602015-01	1
Caelo	Ambroxol hydrochloride	16199603	2
Caelo	Ambroxol hydrochloride	16199602	1
Fagron	Ambroxol hydrochloride	16G12-B06-326184	1
Caelo	Ambroxol hydrochloride	1609002-01	1
Noweda/EuRo	Ambroxol hydrochloride	1609002-02	1
Euro OTC	Ambroxol hydrochloride	1604032-01	1
Euro OTC	Ambroxol hydrochloride	1609002-02	10
Caelo	Ambroxol hydrochloride	170522AH/16309201	1
Caelo	Ambroxol hydrochloride	17002904	1
Euro OTC	Ambroxol hydrochloride	27061702	1
Euro OTC	Ambroxol hydrochloride	1702004-01	5
Caelo	Ambroxol hydrochloride	17158202	1
Caelo	Ambroxol hydrochloride	27101707	1
Euro OTC	Ambroxol hydrochloride	160215-02	1
GEHE	Ambroxol hydrochloride	1702004-02	1
Euro OTC	Ambroxol hydrochloride	170200402	1
Euro OTC	Ambroxol hydrochloride	1702004-02	2
Caelo	Ambroxol hydrochloride	1702004-02	3
Caelo	Ambroxol hydrochloride	17158201	1
Caelo	Ambroxol hydrochloride	17286001	2
Caelo/Gehe	Ambroxol hydrochloride	1702004-02	2
Noweda	Ambroxol hydrochloride	17158201	1
Sanacorp	Ambroxol hydrochloride	170204-02	1
Euro OTC	Ambroxol hydrochloride	1711021-01	6
Sanacorp	Ambroxol hydrochloride	1711021-01	2
Kehr	Ambroxol hydrochloride	18013201	1
Caelo	Ambroxol hydrochloride	18013201	3
Euro OTC	Ambroxol hydrochloride	171102-01	1
Caelo	Ambroxol hydrochloride	1711021-02	1
Caelo	Ambroxol hydrochloride	18013205	1
Caelo	Ambroxol hydrochloride	18013208	1
Euro OTC	Ambroxol hydrochloride	1711021-02	5
Caelo/Gehe	Ambroxol hydrochloride	171158204	1
Euro OTC	Ambroxol hydrochloride	1806009-01	2
Caelo	Ambroxol hydrochloride	1801306	1
Caelo	Ambroxol hydrochloride	18013211	4

- 78 833 spectra from 565 *Apo-Ident* customers from a total of 26 101 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ambroxol hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ambroxol hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 216
Type B	0	380	0	126 512
Type C	0	95	1	78 833

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.8817 %)	98.9583 % (> 95.8333 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22550	22550	0.00	32.29
20742	20742	0.00	31.84
21230	20742	5.04	33.89
21244	22550	4.16	32.93
21942	21942	0.00	30.39
22298	22298	0.00	31.00
22347	22347	0.00	31.46

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Amiloride hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21879-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Amiloride hydrochloride; Amiloridi hydrochloridum dihydricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Amiloride hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Amiloride hydroc...	13J08-B04-288620	21879	40	AR-16-FG-008919-01
Fagron	Amiloride hydroc...	13J08-B04-304547	22339	40	20131024
Fagron	Amiloride hydroc...	16K07-B02-329114	23119	40	20170104

Validation samples

A total of 280317 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 *Amiloride hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 *Amiloride hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Amiloride hydrochloride	13J08-B04-288620	21879 [†]	20
Fagron	Amiloride hydrochloride	13J08-B04-304547	22339 [†]	20
Fagron	Amiloride hydrochloride	15C25-B05-325653	22834	40
Fagron	Amiloride hydrochloride	17F02-B06-335953	23525	40

- 126772 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Amiloride hydrochloride*.

[†]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
Fagron	Amiloride hydrochloride	17J02-B04	1
Fagron	Amiloride hydrochloride	17J02-B04-341175	1

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Amiloride hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Amiloride hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	120	0	126 772
Type C	0	2	0	78 927

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8823 %)	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
23119	21879	23.10	44.39
21879	21879	0.00	43.70
22339	21879	1.70	42.67

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Amitriptyline hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22844-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Amitriptyline hydrochloride; Amitriptylini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Amitriptyline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Amitriptyline hy...	16C31-B01-325540	22844	40	20160425
Inresa	Amitriptyline hy...	005669/17112016	22845	40	1705099
Fagron	Amitriptyline hy...	18A16-B06-348643	24180	40	20180205

Validation samples

A total of 280 317 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 *Amitriptyline hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Amitriptyline hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Inresa	Amitriptyline hydrochloride	005669/06022017	23078	40
Fagron	Amitriptyline hydrochloride	17E11-B02-335098	23528	40

- 126 812 spectra from a total of 2787 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Amitriptyline hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	Amitriptyline hydrochloride	18A16-B06-344853	1
Fagron	Amitriptyline hydrochloride	18A16-B06-348643	1

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Amitriptyline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Amitriptyline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	80	0	126 812
Type C	0	2	0	78 927

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8823 %)	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
22844	22845	14.19	69.38
24180	22845	24.59	67.16
22845	22845	0.00	69.16

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Amphotericin B**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20933-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Amphotericin B; Amphotericinum B

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Amphotericin B*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Amphotericin B	1305033-02	20933	40	1403224
Fagron	Amphotericin B	13I16-N02	21338	40	1508271
Fagron	Amphotericin B	13I16-N02	21951	40	20130911

Validation samples

A total of 280 317 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 *Amphotericin B*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1621 batches from further 372 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 *Amphotericin B*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Amphotericin B	13I16-N02	21951 [†]	20
Euro OTC	Amphotericin B	15I2026-01	22813	40
Fagron	Amphotericin B	16L06-B04-333234	23530	40
Euro OTC	Amphotericin B	1803036	24065	40

- 126 752 spectra from a total of 2785 batches from further 781 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 3 batches from the substance/substance group *Amphotericin B*.

Supplier	Substance	Batch	Spectra
Fagron	Amphotericin B	5173	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
Fagron	Amphotericin B	16D05-B04	1
Euro OTC	Amphotericin B	1305033-03	12

- 78 915 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Amphotericin B* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Amphotericin B* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	128	12	126 752
Type C	0	14	0	78 915

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	91.4286 % (> 89.2857 %)
Type C	100.0000 % (> 99.8818 %)	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
21338	21338	0.00	16.91
21951	21338	6.45	18.12
20933	20933	0.00	13.09

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Arginine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20391-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Arginine; Argininum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Arginine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Arginine	13J28-B02	21226	40	AR-15-FG-008045-01
Euro OTC	Arginine	1604003	22514	40	20160425*
Euro OTC	Arginine	1608031	22801	40	20160916*
Euro OTC	Arginine	1702014	23154	40	20170316*
Fagron	Arginine	16H24-B04-335673	23748	40	20161010

Validation samples

A total of 280 317 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 *Arginine*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1618 batches from further 372 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 3 reference samples from the substance/substance group *Arginine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Arginine	L1405020-01	21712	60
Euro OTC	Arginine	1710010	23774	40
Euro OTC	Arginine	1806010	24154	40

- 126 752 spectra from a total of 2786 batches from further 781 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.

- 52 spectra from 13 *Apo-Ident* customers from 31 batches from the substance/substance group *Arginine*.

*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
Fargon	Arginine	121429	1
Euro OTC	Arginine	1105040-01	1
Euro OTC	Arginine	L1206006-01	1
Fargon	Arginine	13F14-N02	2
Fargon	Arginine	12C21-N04	1
Phönix	Arginine	L1302006-01	1
Fargon	Arginine	13031801	1
Fargon	Arginine	13J28-B02-290463	6
Fargon	Arginine	14B25-B04	2
Caelo	Arginine	13J28-B02-290463	1
Fargon	Arginine	14/24-B08-303720	4
Fargon	Arginine	14I24-B-303720	1
Caelo	Arginine	14I24-B08-303720	1
Fargon	Arginine	14062019	1
Fargon	Arginine	14/24-B08-303901	1
Fargon	Arginine	14092035	2
Fargon	Arginine	1424-B08-303720	1
Euro OTC	Arginine	1604003-01	1
Fargon	Arginine	15C10-B03-318784	1
Fargon	Arginine	14I24-B08-303901	1
Caelo	Arginine	15C10-B03-318785	1
Fargon	Arginine	16D11-B01-322156	1
Fargon	Arginine	15102258	1
Fargon	Arginine	16H24-B04-328914	1
Fargon	Arginine	16H24-B04-335674	7
Fargon	Arginine	16D11-B01-323566	1
Euro OTC	Arginine	1710010-01	2
Fargon	Arginine	16H24-B04-335673	2
Fargon	Arginine	16H24-B04-334063	1
Fargon	Arginine	16032361	1
GEHE	Arginine	17G10-B07-341856	2
Fargon	Arginine	17G10-B07	1

- 78 877 spectra from 565 *Apo-Ident* customers from a total of 26 106 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Arginine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Arginine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	135	5	126 752
Type C	0	52	0	78 877

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	96.4286 % (> 94.2857 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 88.4615 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21226	21226	0.00	54.97
22514	22514	0.00	55.79
22801	22801	0.00	55.58
23154	23154	0.00	55.89
23748	22514	2.39	55.76

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Arginine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20657-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Arginine hydrochloride; Arginini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Arginine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Arginine hydroch...	L1103042-01	20657	40	20110325
Euro OTC	Arginine hydroch...	L1212009-01	20964	40	1402430
Euro OTC	Arginine hydroch...	1306023-01	21776	40	AR-15-FG-008412-01

Validation samples

A total of 280 317 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 *Arginine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Arginine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Arginine hydrochloride	1306023-01	21776 [†]	20
Euro OTC	Arginine hydrochloride	1603033	22512	40
Euro OTC	Arginine hydrochloride	1610042	22877	40
Euro OTC	Arginine hydrochloride	1711014	23875	40
Euro OTC	Arginine hydrochloride	1809012	24313	40

- 126 712 spectra from a total of 2784 batches from further 781 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.

- 17 spectra from 5 *Apo-Ident* customers from 12 batches from the substance/substance group *Arginine hydrochloride*.

[†]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	Arginine hydrochloride	L1212009-01	3
Fagron	Arginine hydrochloride	12C20-M08	1
Euro OTC	Arginine hydrochloride	1306023-01	1
Fagron	Arginine hydrochloride	13j28-b03-287768	1
Fagron	Arginine hydrochloride	13j28-B03-287768	1
Fagron	Arginine hydrochloride	13J28-B032x	1
Fagron	Arginine hydrochloride	13J28-B03	2
EuRho	Arginine hydrochloride	1306023-01	1
Fagron	Arginine hydrochloride	13J28-B03-287766	1
Euro OTC	Arginine hydrochloride	L1407040-01	1
Hirundo Products Vertri...	Arginine hydrochloride	6412784-152	2
Euro OTC	Arginine hydrochloride	L1407040-02	1
Euro OTC	Arginine hydrochloride	L1506023-01	1

- 78 912 spectra from 565 *Apo-Ident* customers from a total of 26 125 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Arginine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Arginine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	180	0	126 712
Type C	0	17	0	78 912

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	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
21776	21776	0.00	42.63
20657	21776	7.25	43.11
20964	20964	0.00	44.24

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ascorbic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20394-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ascorbic acid; Acidum ascorbinicum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ascorbic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ascorbic acid	13G29-B07	21229	40	1410500
Caelo	Ascorbic acid	12350011	21317	40	20121122
Euro OTC	Ascorbic acid	1612018	22918	40	20170109*
Caelo	Ascorbic acid	163452	23062	40	20170125*
Caelo	Ascorbic acid	171358	23293	40	20170524*

Validation samples

A total of 280 317 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 *Ascorbic acid*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1618 batches from further 372 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 9 reference samples from the substance/substance group *Ascorbic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ascorbic acid	1607025	22672	40
Euro OTC	Ascorbic acid	1605024	22680	40
Euro OTC	Ascorbic acid	1609015	22789	40
Euro OTC	Ascorbic acid	1703040	23128	40
Euro OTC	Ascorbic acid	1703025	23144	40
Caelo	Ascorbic acid	171358	23288	40
Euro OTC	Ascorbic acid	1707005	23553	40
Euro OTC	Ascorbic acid	1708026	23701	40
Euro OTC	Ascorbic acid	1710032	23891	40

- 126 532 spectra from a total of 2780 batches from further 781 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.

- 83 spectra from 56 *Apo-Ident* customers from 55 batches from the substance/substance group *Ascorbic acid*.

Supplier	Substance	Batch	Spectra
Wepa	Ascorbic acid	261120415	1
Caelo	Ascorbic acid	2061203	1
Caelo	Ascorbic acid	11208606	1
Caesar & Loretz GmbH	Ascorbic acid	11208606	1
Amos Vital	Ascorbic acid	L1120454	1
Caelo	Ascorbic acid	12349909	1
Caelo	Ascorbic acid	12350003	1
Euro OTC	Ascorbic acid	28081303	1
canea, gehe	Ascorbic acid	VC1242	2
Caelo	Ascorbic acid	12350005	2
Caelo	Ascorbic acid	22101302	1
Caelo	Ascorbic acid	12272601/1	1
Gesundform	Ascorbic acid	L1110704	1
Euro OTC	Ascorbic acid	11121302	1
Euro OTC	Ascorbic acid	L1202011-02	1
Euro OTC	Ascorbic acid	17011404	1
Caelo	Ascorbic acid	12350011	1
Euro OTC	Ascorbic acid	17041406	1
Euro OTC	Ascorbic acid	12061408	1
Caelo	Ascorbic acid	1071404	1
Euro OTC	Ascorbic acid	10071418	1
Caelo	Ascorbic acid	14044701/3	1
Caelo	Ascorbic acid	14123809	2
Wepa Paulus	Ascorbic acid	11406201	1
Caelo	Ascorbic acid	14123910	1
Caelo	Ascorbic acid	14123915	1
ACM	Ascorbic acid	KNC1488J14	6
Caelo	Ascorbic acid	14214403	1
SANACORP	Ascorbic acid	201401318	1
Caelo	Ascorbic acid	13341803/3	1
Gehe/Gehe	Ascorbic acid	L1505001	1
Caelo	Ascorbic acid	15084503	1
Caelo	Ascorbic acid	15084507	1
Caelo	Ascorbic acid	15300002	3
Zentiva/Alliance Health...	Ascorbic acid	15300007	1
Caelo	Ascorbic acid	15359003	1
Caelo	Ascorbic acid	15300007	6
Caelo	Ascorbic acid	153000	1
ACM	Ascorbic acid	Knc1035j16	1
ACM	Ascorbic acid	KNC1035J16	2
Caelo	Ascorbic acid	16050403	3
Caelo	Ascorbic acid	16345202	3
Caelo	Ascorbic acid	123Test	1
Amos Vital GmbH	Ascorbic acid	L1411003	1
GEHE	Ascorbic acid	16345205	1
Caelo	Ascorbic acid	4116E-01016	1
Caelo	Ascorbic acid	12456	1
wepa Apoday	Ascorbic acid	2616110375431	1
Caelo	Ascorbic acid	16345205	3
Caelo	Ascorbic acid	123test	1
Caelo	Ascorbic acid	123456	1
Euro OTC	Ascorbic acid	1710032-01	1
Caelo	Ascorbic acid	17135803	1
Kehr	Ascorbic acid	17360301	1
Amos Vital GmbH/Allianc...	Ascorbic acid	L1711004	1
Caelo	Ascorbic acid	1234567	1

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Supplier	Substance	Batch	Spectra
Caelo	Ascorbic acid	17360301	2
Cealo/Gehe	Ascorbic acid	17360301	1
Caelo	Ascorbic acid	17233201	1
Caelo	Ascorbic acid	17360308	1

- 78 846 spectra from 565 *Apo-Ident* customers from a total of 26 087 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ascorbic 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 *Ascorbic 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	200	0	74 296
Type B	0	360	0	126 532
Type C	0	81	2	78 846

The substance/substance group *Ascorbic 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 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.8817 %)	97.5904 % (> 93.9759 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21229	21229	0.00	63.04
21317	21229	2.51	63.07
22918	22918	0.00	64.75
23062	23062	0.00	63.65
23293	23293	0.00	62.76

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ascorbyl palmitate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21053-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ascorbyl palmitate; Ascorbylis palmitas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ascorbyl palmitate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ascorbyl palmitate	13K04-N01	21053	40	1403226
Fagron	Ascorbyl palmitate	13C06-B40-291206	21665	40	20140306
Fagron	Ascorbyl palmitate	15F01-B99-309774	21851	40	20150615
Fagron	Ascorbyl palmitate	17E18-B06-335527	23520	40	20170606
Fagron	Ascorbyl palmitate	17E18-B06-335527	23520SI	40	20170606

Validation samples

A total of 280317 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 *Ascorbyl palmitate*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1619 batches from further 372 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 *Ascorbyl palmitate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ascorbyl palmitate	13C06-B40-291206	21665 [†]	20
Fagron	Ascorbyl palmitate	15F01-B99-309774	21851 [†]	20
Fagron	Ascorbyl palmitate	17H04-B01-338484	23987	40
Fagron	Ascorbyl palmitate	18A10-B03-344364	24098	40
Fagron	Ascorbyl palmitate	17H04-B01-338484	23987SI	40
Fagron	Ascorbyl palmitate	18A10-B03-344364	24098SI	40

- 126692 spectra from a total of 2785 batches from further 781 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 52 *Apo-Ident* customers from 61 batches from the substance/substance group *Ascorbyl palmitate*.

[†]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
Bionorica	Ascorbyl palmitate	74736	1
Bionorica	Ascorbyl palmitate	74962	1
Bionorica/Noweda	Ascorbyl palmitate	77773	2
PHOENIX 30.06.2014	Ascorbyl palmitate	UQ21206229	1
Fagron	Ascorbyl palmitate	13C06-B40-291206	2
Bionorica Ethics	Ascorbyl palmitate	82275	1
Fagron	Ascorbyl palmitate	14I03-N01	1
Bionorica EthicsGmbH/Sa...	Ascorbyl palmitate	74736	1
Bionorica Ethics7Noweda	Ascorbyl palmitate	82275	2
Bionorica	Ascorbyl palmitate	82275	1
Fagron	Ascorbyl palmitate	K45532790	2
Fagron	Ascorbyl palmitate	15F01-B99	2
Bionorica	Ascorbyl palmitate	85532	1
Bionorica Ethics/ Noweda	Ascorbyl palmitate	85532	2
Fagron	Ascorbyl palmitate	15F01-B99-52063	1
Fagron	Ascorbyl palmitate	15f01-b99-309774	1
Bionorica ethics	Ascorbyl palmitate	85532	2
Fagron	Ascorbyl palmitate	15F01-B99-525122	2
Fagron	Ascorbyl palmitate	16B10-B04-525199	2
Fagron	Ascorbyl palmitate	15F01-B99-525063	1
Fagron	Ascorbyl palmitate	15F01-B99-525121	1
Caelo	Ascorbyl palmitate	16810-B04525199	1
Caelo	Ascorbyl palmitate	15F01-B99-525121	1
Fagron	Ascorbyl palmitate	16B10-B04-525228	1
Caelo	Ascorbyl palmitate	16B10-B04324111	1
Fagron	Ascorbyl palmitate	16I30-B03-525358	2
Fagron	Ascorbyl palmitate	16I30-B03-326543	1
Fagron	Ascorbyl palmitate		1
Fagron	Ascorbyl palmitate	16I30-B03-525380	2
Fagron	Ascorbyl palmitate	16/30-B03	1
Fagron	Ascorbyl palmitate	16I30-B03-329375	1
Fagron	Ascorbyl palmitate	16I30-B03-330625	1
Fagron	Ascorbyl palmitate	16/30-B03-329375	1
Caelo	Ascorbyl palmitate	16B10-B04-525199	1
Caelo	Ascorbyl palmitate	16B-B04-525283	1
Caelo	Ascorbyl palmitate	16I30-B03-525358	2
Fagron	Ascorbyl palmitate	16I30-B03-525426	1
Fagron	Ascorbyl palmitate	16I30-B03-332623	2
Fagron	Ascorbyl palmitate	K47747490	1
Fagron	Ascorbyl palmitate	10061708	1
Euro OTC	Ascorbyl palmitate	16I30-B03	1
Merck	Ascorbyl palmitate	17E18-B06-334914	1
Fagron	Ascorbyl palmitate	16I30-B03	1
Fagron	Ascorbyl palmitate	17E18-B06	1
Fagron	Ascorbyl palmitate	1630-B03-525489	1
Fagron	Ascorbyl palmitate	17E18-B06-525524	3
Fagron	Ascorbyl palmitate	17e18b06334914	1
Fagron	Ascorbyl palmitate	17e18-b06	2
Caelo	Ascorbyl palmitate	17E18-B06-334914	1
Fagron	Ascorbyl palmitate	17H04-B01-338484	6
Bombastus	Ascorbyl palmitate	525526	1
Fagron	Ascorbyl palmitate	525524	1
Fagron	Ascorbyl palmitate	525426	1
Fagron	Ascorbyl palmitate	525489	1
Fagron	Ascorbyl palmitate	525525	1
Fagron	Ascorbyl palmitate	17E18-B06-525514	1
Fagron	Ascorbyl palmitate	17E18-B06-525525	1
Fagron	Ascorbyl palmitate	K48951290	1
Fagron	Ascorbyl palmitate	16L30-B03-332623	1
Fagron	Ascorbyl palmitate	17H04-B01-340474	1

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Supplier	Substance	Batch	Spectra
Fagron	Ascorbyl palmitate	18A10-B03-344364	4
Merck	Ascorbyl palmitate	16130-B03	1
Fagron	Ascorbyl palmitate	23061810	1
Fagron	Ascorbyl palmitate	18B12-B09-525719	2
Fagron	Ascorbyl palmitate	17H04-B01-525632	1
Caelo	Ascorbyl palmitate	18B12-B09-525721	1
Fagron	Ascorbyl palmitate	18B12-B09-525721	1
Fagrin/Noweda	Ascorbyl palmitate	18B12-B09525720	1
Fagron	Ascorbyl palmitate	18B12B09525719	1
Fagron	Ascorbyl palmitate	18B12-B09-348867	1

- 78 834 spectra from 565 *Apo-Ident* customers from a total of 26 076 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ascorbyl 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 *Ascorbyl 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	200	0	74 296
Type B	0	200	0	126 692
Type C	0	92	3	78 834

The substance/substance group *Ascorbyl 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 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8817 %)	96.8421 % (> 93.6842 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21053	21053	0.00	62.50
21665	21053	18.12	54.59
21851	21053	20.48	55.06
23520	21053	15.00	58.85

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Atropine sulfate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20653-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Atropine sulfate; Atropine sulphate; Atropini sulfas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Atropine sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Atropine sulfate	11180602	20653	30	1405538
Caelo	Atropine sulfate	13173808	21088	40	1403483
Caelo	Atropine sulfate	13357405	21551	50	1504594
Caelo	Atropine sulfate	14336806	21719	40	1510209
Caelo	Atropine sulfate	15301601	21920	40	20150930
Caelo	Atropine sulfate	14336806	21719SI	40	1510209
Caelo	Atropine sulfate	15301601	21920SI	40	20150930

Validation samples

A total of 280317 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 *Atropine sulfate*. These samples are listed above in the [calibration samples](#) section.
- 74216 spectra from a total of 1618 batches from further 372 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 [†].

- 390 spectra of 12 reference samples from the substance/substance group *Atropine sulfate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Atropine sulfate	14336806	21719 [†]	20
Caelo	Atropine sulfate	15301601	21920 [†]	20
Fagron	Atropine sulfate	16G20-B06-328437	22932	40
Caelo	Atropine sulfate	16326802	22952	40
Caelo	Atropine sulfate	170264	23367	40
Caelo	Atropine sulfate	172732	23682	40
Caelo	Atropine sulfate	14336806	21719SI [†]	20
Caelo	Atropine sulfate	15301601	21920SI [†]	20
Fagron	Atropine sulfate	16G20-B06-328437	22932SI	40
Caelo	Atropine sulfate	16326802	22952SI	40
Caelo	Atropine sulfate	170264	23367SI	40
Caelo	Atropine sulfate	172732	23682SI	30

- 126502 spectra from a total of 2783 batches from further 781 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](#).

[†]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.

- 14 spectra from 11 *Apo-Ident* customers from 10 batches from the substance/substance group *Atropine sulfate*.

Supplier	Substance	Batch	Spectra
Noweda	Atropine sulfate	12250403	1
fargon	Atropine sulfate	13K01-N01	1
Caelo	Atropine sulfate	13173809	1
Caelo	Atropine sulfate	13357403	1
Caelo	Atropine sulfate	13357405	1
Caelo	Atropine sulfate	14336807	1
Caelo	Atropine sulfate	15115201	3
Phönix	Atropine sulfate	15301607	1
Caelo	Atropine sulfate	16c15b03-319166	1
Gehe	Atropine sulfate	16326802	1
Caelo	Atropine sulfate	16326802	2

- 78 915 spectra from 565 *Apo-Ident* customers from a total of 26 127 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Atropine sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Atropine sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 216
Type B	0	390	0	126 502
Type C	0	14	0	78 915

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.4615 %)
Type C	100.0000 % (> 99.8818 %)	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
20653	20653	0.00	33.80
21088	21088	0.00	33.92
21551	21551	0.00	32.31
21719	21719	0.00	33.57
21920	21719	11.92	40.16

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Bacitracin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20851-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Bacitracin; Bacitracinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Bacitracin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Bacitracin	13A-03-N11	20851	20	1401189
Fagron	Bacitracin	14A21-B09-292909	21657	40	1511741
Roth	Bacitracin	194169081	21658	40	20140508
Fagron	Bacitracin	14E23-B03-296243	21686	30	1503715
Fagron	Bacitracin	15C12-B06-309185	21898	40	20150324

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Bacitracin	15C12-B06-309185	21986	40	9466
Fagron	Bacitracin	16B17-B03-322939	22739	40	20160421
Fagron	Bacitracin	17L11-B02-343685	23933	40	1806068

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 290 spectra of 8 reference samples from the substance/substance group *Bacitracin*. These samples are listed above in the [calibration samples](#) section.
- 74206 spectra from a total of 1616 batches from further 372 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 [†].

- 410 spectra of 11 reference samples from the substance/substance group *Bacitracin*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Bacitracin	13A-03-N11	20851 [†]	20
Fagron	Bacitracin	14A21-B09-292909	21657 [†]	20
Roth	Bacitracin	194169081	21658 [†]	20
Fagron	Bacitracin	14E23-B03-296243	21686 [†]	30
Fagron	Bacitracin	15C12-B06-309185	21898 [†]	20
Fagron	Bacitracin	15C12-B06-309185	21986 [†]	20
Fagron	Bacitracin	16I12-B03-334194	23531	40
Fagron	Bacitracin	14A21-B09-292909	21657SI	60
Fagron	Bacitracin	14E23-B03-296243	21686SI	60
Fagron	Bacitracin	15C12-B06-309185	21898SI	60
Fagron	Bacitracin	15C12-B06-309185	21986SI	60

- 126482 spectra from a total of 2783 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the

[†]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.

- 76 spectra from 50 *Apo-Ident* customers from 44 batches from the substance/substance group *Bacitracin*.

Supplier	Substance	Batch	Spectra
Fagron	Bacitracin	11J17-N01	2
Fagron	Bacitracin	211531	1
Fagron	Bacitracin	12G12-N17	1
Fagron	Bacitracin	13A03-N11	1
Fagron	Bacitracin	13D26-N08	1
Fagron	Bacitracin	13C13-N10	1
Fagron	Bacitracin	13B25-B01	1
Fagron	Bacitracin	14A21-B09-290643	2
Fagron	Bacitracin	14A21-B09-290645	2
Fagron	Bacitracin	14A21-B09	2
Fagron	Bacitracin	14A21-B09-292908	1
Fagron	Bacitracin	C2280017	3
Fagron	Bacitracin	14E23-B03-296243	6
Fagron	Bacitracin	14E23-B03-296245	2
Caelo	Bacitracin	14E23-B03-296243	2
Caelo	Bacitracin	14A21-B09-292908	1
Phönix Gotha	Bacitracin	C2280010	1
Fagron	Bacitracin	14E23-B03-333424	1
Fagraon	Bacitracin	14E23-B03-303424	1
Fagron	Bacitracin	14E23-B03-303424	2
Fagron	Bacitracin	14E23-B03	3
Fagron	Bacitracin	14E23B03-303424	1
Fagron	Bacitracin	14e23-b03-296243	1
Fargon/Phönix	Bacitracin	15C12-B06-312975	1
Caelo	Bacitracin	15C12-B06-317782	1
Fagron	Bacitracin	15C12-B06-317782	1
Fagron	Bacitracin	15C12-B06	1
Fagron	Bacitracin	16B17-B03-322891	4
Fagron	Bacitracin	16B17-B03	2
Gehe	Bacitracin	C2280065	1
Fagron	Bacitracin	C2280065	2
Fagron	Bacitracin	16I12-B03-329401	1
Fagron	Bacitracin	16b17-b03-322939	1
Fagron	Bacitracin	16/12-B03-329401	1
Fagron	Bacitracin	16/12-B03-331152	1
Fagron	Bacitracin	16I12-B03-334052	2
Caelo	Bacitracin	16I12-B03-331152	1
Fagron	Bacitracin	16I12-B03	2
Fagron	Bacitracin	2917M-03314	1
Fagron	Bacitracin		1
Fagron	Bacitracin	16I12-B03-335331	1
Phönix	Bacitracin	c2280065	1
Fagron	Bacitracin	1612-B033-334052	1
Fargon/Gehe	Bacitracin	C2280092	1
Fagron	Bacitracin	17L11-B02	2
Fagron	Bacitracin	17L11-B02-343685	2
Fagron	Bacitracin	17L11-B02-343686	1

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Supplier	Substance	Batch	Spectra
Kehr	Bacitracin	16B17-B03-322891	1
AHD	Bacitracin	17L11-B02-344244	1
Euro OTC	Bacitracin	17L11-B02-348461	1
Caelo	Bacitracin	C2280092	1

- 78 853 spectra from 565 *Apo-Ident* customers from a total of 26 093 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Bacitracin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bacitracin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 206
Type B	0	381	29	126 482
Type C	0	75	1	78 853

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.9310 %)
Type B	100.0000 % (> 99.9901 %)	92.9268 % (> 92.1951 %)
Type C	100.0000 % (> 99.8817 %)	98.6842 % (> 94.7368 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
20851	20851	0.00	17.68
21986	21986	0.00	29.09
21657	21657	0.00	22.67
21658	21986	2.61	25.34
22739	23933	4.39	24.30
23933	23933	0.00	16.92
21686	21686	0.00	10.36
21898	21986	3.22	23.10

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Beclometasone dipropionate, anhydrous
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	21046-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Beclometasone dipropionate, anhydrous; Beclometasoni dipropionas anhydricus

Special notes

When selecting the *Beclometasone dipropionate, anhydrous* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Beclometasone dipropionate, anhydrous*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Beclometasone di...	13I05-N03	21046	60	1511689
Fagron	Beclometasone di...	13E02-B40-293328	21554	40	20140508
Euro OTC	Beclometasone di...	1203022-03	21634	25	1509281
Fagron	Beclometasone di...	13E02-B40-296353	21977	40	20140508
Euro OTC	Beclometasone di...	1502032	22989	40	20150327*
Fagron	Beclometasone di...	13E02-B40-296353	21977SI	20	20140508
Euro OTC	Beclometasone di...	1502032	22989SI	30	20150327*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 255 spectra of 7 reference samples from the substance/substance group *Beclometasone dipropionate, anhydrous*. These samples are listed above in the [calibration samples](#) section.
- 74 241 spectra from a total of 1618 batches from further 372 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 [†].

- 277 spectra of 9 reference samples from the substance/substance group *Beclometasone dipropionate, anhydrous*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Beclometasone dipropionate, ...	1203022-03	21634 [†]	35
Fagron	Beclometasone dipropionate, ...	13E02-B40-296353	21977 [†]	20
Euro OTC	Beclometasone dipropionate, ...	1203022-03	21995	60
Fagron	Beclometasone dipropionate, ...	15F29-B09-314376	23104	40
Fagron	Beclometasone dipropionate, ...	16B16-B03-342082	23930	40
Fagron	Beclometasone dipropionate, ...	13E02-B40-296353	21977SI [†]	9
Euro OTC	Beclometasone dipropionate, ...	1203022-03	21995SI	28
Fagron	Beclometasone dipropionate, ...	15F29-B09-314376	23104SI	20
Fagron	Beclometasone dipropionate, ...	16B16-B03-342082	23930SI	25

- 126 615 spectra from a total of 2785 batches from further 781 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.

- 37 spectra from 15 *Apo-Ident* customers from 21 batches from the substance/substance group *Beclometasone dipropionate, anhydrous*.

Supplier	Substance	Batch	Spectra
Fagron	Beclometasone dipropionate, ...	11L01-N03	1
Fagron	Beclometasone dipropionate, ...	12D12-N03	4
Fagron	Beclometasone dipropionate, ...	11F28-N02	2
Fagron	Beclometasone dipropionate, ...	12G04-N11	3
Euro OTC	Beclometasone dipropionate, ...	1203022-01	2
fragon	Beclometasone dipropionate, ...	700721-0004	1
Fagron	Beclometasone dipropionate, ...	13E02-B40-293328	2
Fagron	Beclometasone dipropionate, ...	13I05-N03	3
Fagron	Beclometasone dipropionate, ...	13I05N03	1
Fagron	Beclometasone dipropionate, ...	13E02-B40-296354	2
Fagron	Beclometasone dipropionate, ...	13E02-B40-293327	3
Fagron	Beclometasone dipropionate, ...	13/05-N03	1
Euro OTC	Beclometasone dipropionate, ...	1203022-03	1
Fagron	Beclometasone dipropionate, ...	14D04-B04-302336	3
Fagron	Beclometasone dipropionate, ...	13/05-N03	1
Fagron	Beclometasone dipropionate, ...	14D04-B04-302335	1
Euro OTC	Beclometasone dipropionate, ...	C0783111020	1
Fagron	Beclometasone dipropionate, ...	16B16-B03-318877	1
Fagron	Beclometasone dipropionate, ...	16B16-B03-322517	1
Euro OTC	Beclometasone dipropionate, ...	1502032-02	1
Fagro/Noweda	Beclometasone dipropionate, ...	14D04-B04-302335	1
Fagron	Beclometasone dipropionate, ...	18C05-B01-347367	1

- 78 892 spectra from 565 *Apo-Ident* customers from a total of 26 116 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	255	0	74 241
Type B	0	277	0	126 615
Type C	0	36	1	78 892

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.6471 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.8339 %)
Type C	100.0000 % (> 99.8817 %)	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
21554	22989	2.03	27.72
22989	22989	0.00	29.18
21046	21046	0.00	29.38
21977	21634	4.21	26.85
21634	21634	0.00	28.13

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Benzocaine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20211-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Benzocaine; Benzocainum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Benzocaine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzocaine	12341904	20843	40	1411055
Caelo	Benzocaine	13213509	21563	40	1706017
Fagron	Benzocaine	16D13-B01-342411	23986	40	1807429

Validation samples

A total of 280317 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 *Benzocaine*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 [†].

- 210 spectra of 6 reference samples from the substance/substance group *Benzocaine*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Benzocaine	12E04-N06	21083	30
Caelo	Benzocaine	13213509	21563 [†]	20
Caelo	Benzocaine	161740	22641	40
Fagron	Benzocaine	14G02-B01-306980	23569	40
Caelo	Benzocaine	172174	23628	40
Caelo	Benzocaine	182778	24378	40

- 126682 spectra from a total of 2783 batches from further 781 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.

- 200 spectra from 130 *Apo-Ident* customers from 90 batches from the substance/substance group *Benzocaine*.

[†]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	Benzocaine	11127506	1
Fagron	Benzocaine	12E04-N06	9
Caelo	Benzocaine	11127508	1
Caelo	Benzocaine	12115007	4
Fagron	Benzocaine	10K02-N01	1
Caelo	Benzocaine	12115008	2
Caelo	Benzocaine	91062169	1
s.Prüfprotokoll	Benzocaine		1
Phoenix	Benzocaine	12H10-N06	1
Fagron	Benzocaine	BZ-08/11-12	1
Caelo	Benzocaine	19031301	1
Fagron	Benzocaine	11/22-N3	1
Caelo	Benzocaine	12115011	3
Fagron	Benzocaine	11/22-N03	1
Fargon	Benzocaine	12H10-N06	1
Caelo	Benzocaine	12341904	5
Caelo	Benzocaine	10072603	2
Phönix	Benzocaine	13F06-N10	1
Fagron	Benzocaine	BZ-27/1112	1
Fagron	Benzocaine	12H10-N06	3
Caelo	Benzocaine	12341906	1
Fagron	Benzocaine	13F06-N10	1
Fagron	Benzocaine	12341904	1
Caelo	Benzocaine	5021401	1
Caelo	Benzocaine	13213502	5
Fargon/Sana	Benzocaine	11K08-290049	1
Fagron	Benzocaine	11K08-B40	4
Sanacorp	Benzocaine	13213502	1
Caelo	Benzocaine	3784947	1
Caelo	Benzocaine	13213509	6
Fagron	Benzocaine	104210-0001	1
Fagron	Benzocaine	11k08-B40-291841	1
Fagron	Benzocaine	11K08-B40-291841	4
Fagron	Benzocaine	4413E-01118	1
Fagron	Benzocaine	11K08-B40-291840	1
Anzag / Noweda	Benzocaine	1321351	1
Fagron	Benzocaine	11k08-b40-291841	1
Fargon	Benzocaine	13L06-B02-294112	1
Fagron	Benzocaine	13L06-B02	4
Caelo	Benzocaine	6031501	1
Caelo	Benzocaine	2412M-01118	1
Fagron	Benzocaine	13L06-B02-294112	2
Caelo	Benzocaine	13L06-B02-294112	1
Sanacorp	Benzocaine	13213506	1
Caelo	Benzocaine	13213515	2
Caelo	Benzocaine	14277502	4
Fagron	Benzocaine	13L06-B02297505	1
Fagron	Benzocaine	400313	1
Caelo	Benzocaine	13213516	1
Caelo	Benzocaine	13213518	1
Fagron	Benzocaine	13L06-B02-294100	2
Fagron	Benzocaine	13L06-B02-300494	3
Fagron	Benzocaine	13L06Bo2	1
Caelo	Benzocaine	15227302	7
Caelo	Benzocaine		1
Euro OTC	Benzocaine	13L06-B02-297505	1
Fagron	Benzocaine	13106-B02-300494	1
Fagron	Benzocaine	14G02-B01-310324	6
ACM	Benzocaine	KNC1643J15	1
Caelo	Benzocaine	1515I-01118	1

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Supplier	Substance	Batch	Spectra
Caelo	Benzocaine	15227307	4
Fagron	Benzocaine	15227307	1
Fagron	Benzocaine	15C19-B04-308254	1
Fagron	Benzocaine	15C19-B04-316239	2
Fagron	Benzocaine	15C19-B04	1
Caelo	Benzocaine	15227311	2
Caelo	Benzocaine	15227314	3
Fagron	Benzocaine	12E014-N06	1
Caelo	Benzocaine	15227315	4
Fagron	Benzocaine	15C19-B04-322019	5
Caelo	Benzocaine	15227317	1
Gehe	Benzocaine	111214	1
Caelo	Benzocaine	16174001	4
Euro OTC	Benzocaine	15227313	1
Caelo	Benzocaine	11031703	1
Gehe	Benzocaine	15C19-B04	1
Caelo	Benzocaine	16030403	1
AHD	Benzocaine	16174001	1
Fagron	Benzocaine	14G02-B01-318318	1
Fagron	Benzocaine	14G02B01318318	1
Kehr	Benzocaine	15C19-B04-325359	1
Caelo	Benzocaine	15C19-B04-322019	1
Kehr	Benzocaine	16D13-B01-330168	1
Fagron	Benzocaine	15C19-B04-325359	2
Caelo	Benzocaine	16174007	6
Caelo	Benzocaine	15227313	1
Caelo	Benzocaine	16174014	5
Fagron	Benzocaine	16D13-B01-330168	1
Caelo	Benzocaine	161740075429	1
Caelo	Benzocaine	16174019	4
Caelo	Benzocaine	161740195459	1
Sanacorp W.E:07.01.14 ...	Benzocaine	13213502	1
Fagron	Benzocaine	16D13	1
Caelo	Benzocaine	18041803	1
Fagron	Benzocaine	16D13-B01	1
Fagron	Benzocaine	16D13-B01-337264	1
Fiebig	Benzocaine	18018801	1
Caelo	Benzocaine	18018801	4
Fagron	Benzocaine	16D13-B01-345969	1
Fagron	Benzocaine	16D13-B01-342411	1
Caelo	Benzocaine	16174017	1
Caelo	Benzocaine	16D13-B01-345969	1
Fagron	Benzocaine	16D13-B01-348062	1
Caelo	Benzocaine	18018804	3
Fagron	Benzocaine	16D13-B01-334195	1
Fagron	Benzocaine	18F18-B50-352167	1
Fagron	Benzocaine	18F18-B50-352171	1

- 78 729 spectra from 565 *Apo-Ident* customers from a total of 26 049 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Benzocaine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Benzocaine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	180	30	126 682
Type C	0	170	30	78 729

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	85.7143 % (> 84.2857 %)
Type C	100.0000 % (> 99.8817 %)	85.0000 % (> 83.5000 %)

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
20843	20843	0.00	90.17
21563	21563	0.00	91.12
23986	23986	0.00	91.51

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Benzoic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20041-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Benzoic acid; Acidum benzoicum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Benzoic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzoic acid	13391310	21458	40	20131216
Caelo	Benzoic acid	15084611	23095	40	20150318
Caelo	Benzoic acid	15084614	23096	40	1707644

Validation samples

A total of 280 317 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 *Benzoic acid*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Benzoic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Benzoic acid	13391310	21458 [†]	20
Caelo	Benzoic acid	15084614	22664	40
Caelo	Benzoic acid	15084614	23726	40
Caelo	Benzoic acid	162701	24027	40

- 126 752 spectra from a total of 2786 batches from further 781 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 21 *Apo-Ident* customers from 19 batches from the substance/substance group *Benzoic acid*.

Supplier	Substance	Batch	Spectra
Caelo	Benzoic acid	10156104	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
Phönix	Benzoic acid	13074605	2
Caelo	Benzoic acid	13074605	2
Caelo	Benzoic acid	13391310	1
Caelo	Benzoic acid	13074610	4
Gatt-Koller / Phoenix	Benzoic acid	2992/07131314	2
Caelo	Benzoic acid	13391314	1
Caelo	Benzoic acid	13391320	1
Caelo	Benzoic acid	1339120	1
Caelo	Benzoic acid	15084701	1
Fresenius	Benzoic acid	80715102	1
Caelo	Benzoic acid	15084603	3
Caelo	Benzoic acid	15084607	3
ACM	Benzoic acid	KNC0558J15	1
Caleo/Phoenix	Benzoic acid	15084607	1
Anza	Benzoic acid	16001702	1
Anzag	Benzoic acid	16001708	1
ACM	Benzoic acid	KNC0396J17	1
Caelo	Benzoic acid	16001714	3
Caelo	Benzoic acid	1732701	1
Caelo	Benzoic acid	17327101	1

- 78 896 spectra from 565 *Apo-Ident* customers from a total of 26 118 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Benzoic 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 *Benzoic 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	120	0	74 376
Type B	0	140	0	126 752
Type C	0	30	3	78 896

The substance/substance group *Benzoic 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 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.8817 %)	90.9091 % (> 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
21458	23096	12.16	38.40
23095	23096	10.15	39.38
23096	23096	0.00	44.10

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Benzydamine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20624-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Benzydamine hydrochloride; Benzydamini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Benzydamine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Benzydamine hydr...	14I30-B04-300713	21699	30	AR-15-FG-015977-01
Fagron	Benzydamine hydr...	15I17-B02-315060	22268	40	20151211
Fagron	Benzydamine hydr...	16D05-B50-332333	23203	40	20170323
Audor	Benzydamine hydr...	AP300111801004B	24411	40	20180418

Validation samples

A total of 280317 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 *Benzylamine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74346 spectra from a total of 1619 batches from further 372 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 [†].

- 115 spectra of 4 reference samples from the substance/substance group *Benzylamine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Benzylamine hydrochloride	14I30-B04-300713	21699 [†]	15
Fagron	Benzylamine hydrochloride	15I17-B02-315060	22268 [†]	20
Fagron	Benzylamine hydrochloride	16D05-B50-332333	23204	40
Fagron	Benzylamine hydrochloride	17H01-B03-345050	23942	40

- 126777 spectra from a total of 2785 batches from further 781 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 29 *Apo-Ident* customers from 27 batches from the substance/substance group *Benzylamine hydrochloride*.

[†]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
Fagron	Benzydamine hydrochloride	13H19N06	1
Fagron	Benzydamine hydrochloride	13A15-N03	1
Fagron	Benzydamine hydrochloride	12K07-N16	1
Fagron	Benzydamine hydrochloride	12C20-N02	1
Fagron	Benzydamine hydrochloride	14B25-B01-294054	1
Fresenius	Benzydamine hydrochloride	30062015099	1
Fagron	Benzydamine hydrochloride	15A14-B05-303068	1
Fagron	Benzydamine hydrochloride	1503309P	1
Fagron	Benzydamine hydrochloride	16B09-B05-318272	2
Fagron	Benzydamine hydrochloride	16B09-B05-320007	1
Fagron	Benzydamine hydrochloride	15I17-B02	1
Fagron	Benzydamine hydrochloride	15A14-B05	1
Fagron	Benzydamine hydrochloride	1503313P	1
Fagron	Benzydamine hydrochloride	13H19-N06	1
Fagron	Benzydamine hydrochloride	25021710	1
Fagron	Benzydamine hydrochloride	12J10-N03	1
Fagron	Benzydamine hydrochloride	3280417	1
Fagron	Benzydamine hydrochloride	16D05-b50-332334	1
Fagron	Benzydamine hydrochloride		1
Caelo	Benzydamine hydrochloride	12K07-N16	1
Fagron	Benzydamine hydrochloride	16D05-B50-332334	1
Audor Pharma	Benzydamine hydrochloride	300111702007B	1
Audor Pharma	Benzydamine hydrochloride	AP300111702007B	3
Audor Pharma	Benzydamine hydrochloride	300111702007b	1
Fagron	Benzydamine hydrochloride	1703305P	1
Fagron	Benzydamine hydrochloride	17H01-B03-345050	2
Caelo	Benzydamine hydrochloride	17H01-B03-345050	1
Fagron	Benzydamine hydrochloride	17H01-B0334641	1
Fagron	Benzydamine hydrochloride	17H01-B03-345051	1

- 78 896 spectra from 565 *Apo-Ident* customers from a total of 26 110 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Benzydamine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Benzydamine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 346
Type B	0	115	0	126 777
Type C	0	33	0	78 896

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.7826 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 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
21699	21699	0.00	40.38
22268	21699	3.11	40.23
23203	21699	3.91	41.47
24411	21699	11.89	41.41

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Betaine monohydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20498-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Betaine monohydrate; Betainum monohydricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Betaine monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Betaine monohydr...	12336602	20991	40	1403327
Fagron	Betaine monohydr...	14I26-B06-309878	21956	40	20141212

Validation samples

A total of 280 317 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 *Betaine monohydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Betaine monohydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Betaine monohydrate	14I26-B06-309878	21956 [†]	20
Fagron	Betaine monohydrate	16H03-B04-330370	23092	40
Fagron	Betaine monohydrate	16H03-B04-330370	23378	40

- 126 792 spectra from a total of 2787 batches from further 781 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 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Betaine monohydrate*.

Supplier	Substance	Batch	Spectra
Caelo	Betaine monohydrate	4312172831	1
Fagron	Betaine monohydrate	16H03-B04-330370	1
Caelo	Betaine monohydrate	14A14-B02-292983	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*.

- 78 926 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Betaine monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Betaine monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	100	0	126 792
Type C	0	3	0	78 926

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8821 %)	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
20991	20991	0.00	56.77
21956	20991	4.37	59.46

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Betamethasone dipropionate, micronized
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20930-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Betamethasone dipropionate, micronized; Betamethasoni dipropionas micronisatum

Special notes

When selecting the *Betamethasone dipropionate, micronized* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Betamethasone dipropionate, micronized*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Betamethasone di...	13I17-N05	20930	40	1401377
Caelo	Betamethasone di...	13372501	21250	40	AR-15-FG-005428-01
Caelo	Betamethasone di...	13236803	21366	50	20130730
Euro OTC	Betamethasone di...	1311023-01	21716	40	1505455
Euro OTC	Betamethasone di...	1601034	22372	30	20160204*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Betamethasone di...	16C04-B03-324513	22898	40	20160421
Caelo	Betamethasone di...	13372501	21250SI	30	AR-15-FG-005428-01
Caelo	Betamethasone di...	13236803	21366SI	31	20130730
Euro OTC	Betamethasone di...	1311023-01	21716SI	30	1505455
Euro OTC	Betamethasone di...	1601034	22372SI	30	20160204*
Fagron	Betamethasone di...	16C04-B03-324513	22898SI	39	20160421

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 11 reference samples from the substance/substance group *Betamethasone dipropionate, micronized*. These samples are listed above in the [calibration samples](#) section.
- 74 096 spectra from a total of 1617 batches from further 372 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 [†].

- 687 spectra of 21 reference samples from the substance/substance group *Betamethasone dipropionate, micronized*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Betamethasone dipropionate, ...	13I17-N05	20952	80
Caelo	Betamethasone dipropionate, ...	13236803	21367	40
Euro OTC	Betamethasone dipropionate, ...	1311023-01	21716 [†]	20
Euro OTC	Betamethasone dipropionate, ...	1601034	22372 [†]	15
Euro OTC	Betamethasone dipropionate, ...	1610014	22851	40
Caelo	Betamethasone dipropionate, ...	171059	23342	40
Euro OTC	Betamethasone dipropionate, ...	1705020	23539	40
Caelo	Betamethasone dipropionate, ...	173536	23839	40
Euro OTC	Betamethasone dipropionate, ...	1801045	24090	40
Euro OTC	Betamethasone dipropionate, ...	1811007	24343	40
Caelo	Betamethasone dipropionate, ...	13372501	21250SI [†]	15
Caelo	Betamethasone dipropionate, ...	13236803	21366SI [†]	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	Betamethasone dipropionate, ...	13236803	21367SI	60
Euro OTC	Betamethasone dipropionate, ...	1311023-01	21716SI [†]	16
Euro OTC	Betamethasone dipropionate, ...	1601034	22372SI [†]	15
Euro OTC	Betamethasone dipropionate, ...	1610014	22851SI	30
Caelo	Betamethasone dipropionate, ...	171059	23342SI	20
Euro OTC	Betamethasone dipropionate, ...	1705020	23539SI	27
Caelo	Betamethasone dipropionate, ...	173536	23839SI	25
Euro OTC	Betamethasone dipropionate, ...	1801045	24090SI	39
Euro OTC	Betamethasone dipropionate, ...	1811007	24343SI	30

- 126 205 spectra from a total of 2778 batches from further 781 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.

- 457 spectra from 202 *Apo-Ident* customers from 141 batches from the substance/substance group *Betamethasone dipropionate, micronized*.

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone dipropionate, ...	12827-N08	1
Fagron	Betamethasone dipropionate, ...	10E19-N03	1
Fagron	Betamethasone dipropionate, ...	12B27-N08	4
Fagron	Betamethasone dipropionate, ...	9J05-N09	1
Fagron	Betamethasone dipropionate, ...	11K28-N10	2
Fagron	Betamethasone dipropionate, ...	11D26-N06	2
Caelo	Betamethasone dipropionate, ...	12114506	1
Euro OTC	Betamethasone dipropionate, ...	12114511	2
Caelo	Betamethasone dipropionate, ...	12114507	2
Caelo	Betamethasone dipropionate, ...	12114512	1
Fagron	Betamethasone dipropionate, ...	12C21-N13	1
Anzag	Betamethasone dipropionate, ...	12114513	2
Caelo	Betamethasone dipropionate, ...	1210020-01	1
Euro OTC	Betamethasone dipropionate, ...	121002001	1
Caelo	Betamethasone dipropionate, ...	13023001	3
Bombastus	Betamethasone dipropionate, ...	12B27N08	1
Euro OTC	Betamethasone dipropionate, ...	1303006/01	1
Fagron	Betamethasone dipropionate, ...	13023004	1
Caelo	Betamethasone dipropionate, ...	13023005	7
Caelo	Betamethasone dipropionate, ...	13023002	5
Euro OTC	Betamethasone dipropionate, ...	1303006-01	2
EUro/AHD	Betamethasone dipropionate, ...	1303006-01	3
Caelo	Betamethasone dipropionate, ...	12114501	1
Hirsch	Betamethasone dipropionate, ...	1303006-01	1
Caelo	Betamethasone dipropionate, ...		1
Euro OTC	Betamethasone dipropionate, ...	1303006-02	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	Betamethasone dipropionate, ...	1325702	1
Caelo	Betamethasone dipropionate, ...	13125701	3
Euro OTC	Betamethasone dipropionate, ...	1305041-01	9
Caelo	Betamethasone dipropionate, ...	13125703	4
Euro OTC	Betamethasone dipropionate, ...	130541-01	1
Caelo	Betamethasone dipropionate, ...	13236801	6
Cealo/Sanacorp	Betamethasone dipropionate, ...	13125701	1
Noweda	Betamethasone dipropionate, ...	13236802	1
Fagron	Betamethasone dipropionate, ...	13I17-N05	11
Euro OTC	Betamethasone dipropionate, ...	13125702	1
Caelo	Betamethasone dipropionate, ...	AKD11	1
Fagron	Betamethasone dipropionate, ...		4
Fagron	Betamethasone dipropionate, ...	13/17-N05	13
Euro OTC	Betamethasone dipropionate, ...	1305041-02	3
Caelo	Betamethasone dipropionate, ...	13236802	4
Fagron	Betamethasone dipropionate, ...	8K03-N13	2
Caelo	Betamethasone dipropionate, ...	13236805	3
Caelo	Betamethasone dipropionate, ...	12114513	1
Alliance Health 24.01.2...	Betamethasone dipropionate, ...	13/17-N05	1
Phoenix	Betamethasone dipropionate, ...	13236806	1
Caelo	Betamethasone dipropionate, ...	13236801ok	1
Caelo	Betamethasone dipropionate, ...	13236806	3
Euro OTC	Betamethasone dipropionate, ...	1311023-01	5
Caelo	Betamethasone dipropionate, ...	13372501	3
Phoenix 03.04.20147	Betamethasone dipropionate, ...	13236805	1
Caelo	Betamethasone dipropionate, ...	140507	1
Euro OTC	Betamethasone dipropionate, ...	13372501	1
Fagron	Betamethasone dipropionate, ...	1317-N05	1
Euro OTC	Betamethasone dipropionate, ...	131102301	2
Caelo	Betamethasone dipropionate, ...	1303006-01	1
Noweda	Betamethasone dipropionate, ...	13236803	1
Caelo	Betamethasone dipropionate, ...	13372504	5
Caelo	Betamethasone dipropionate, ...	13236803	1
Caelo	Betamethasone dipropionate, ...	13372503	7
	Betamethasone dipropionate, ...	13/17-N05	2
Caelo	Betamethasone dipropionate, ...	13372514	9
Caelo	Betamethasone dipropionate, ...	13372515	3
Caelo	Betamethasone dipropionate, ...	13372516	4
Fagron	Betamethasone dipropionate, ...	14C03-B06-296837	6
Euro OTC	Betamethasone dipropionate, ...	1311023-02	4
Fagron	Betamethasone dipropionate, ...	13j16-B01-291844	1
Euro OTC	Betamethasone dipropionate, ...	1503003-01	8
Fagron	Betamethasone dipropionate, ...	13/17-n05	1
Fagron	Betamethasone dipropionate, ...	13J16-B01-291845	1
Caelo	Betamethasone dipropionate, ...	13/17-N05	2
Caelo	Betamethasone dipropionate, ...	15163301	13
Caelo	Betamethasone dipropionate, ...	15163302	5
Caelo	Betamethasone dipropionate, ...	13372520	1
Caelo	Betamethasone dipropionate, ...	15163303	10
Caelo	Betamethasone dipropionate, ...	1503003-01	2
Caelo	Betamethasone dipropionate, ...	14C03-B06-296837	1
Euro OTC	Betamethasone dipropionate, ...	1503003-02	7
Caelo	Betamethasone dipropionate, ...	2109DM0B00111322	1
Caelo	Betamethasone dipropionate, ...	13372512	1
Euro/Sanacorp	Betamethasone dipropionate, ...	1503003-02	1
WE:09.12.2016	Betamethasone dipropionate, ...	15163301	1
Fagron	Betamethasone dipropionate, ...	14C03-B03-296838	1
WE:05.04.2016 Phönix	Betamethasone dipropionate, ...	15163304	4
Caelo	Betamethasone dipropionate, ...	1503003-02	1
Caelo	Betamethasone dipropionate, ...	15163204	1

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Supplier	Substance	Batch	Spectra
Fargon/ Noweda	Betamethasone dipropionate, ...	13/17-N05	1
Euro OTC	Betamethasone dipropionate, ...	160103401	1
Euro OTC	Betamethasone dipropionate, ...	1601034-01	19
Euro OTC	Betamethasone dipropionate, ...	1506016-02	1
Euro OTC	Betamethasone dipropionate, ...	150300302	1
Caelo	Betamethasone dipropionate, ...	15163305	1
Caelo	Betamethasone dipropionate, ...	15412901	1
Fagron	Betamethasone dipropionate, ...	15H25-B06-313088	1
Fagron	Betamethasone dipropionate, ...	15H28-B06-313088	2
Euro/Gehe	Betamethasone dipropionate, ...	1601034-01	1
Euro OTC	Betamethasone dipropionate, ...	15163304	1
Caelo	Betamethasone dipropionate, ...	15163304	6
Caelo	Betamethasone dipropionate, ...	15238701	19
Caelo	Betamethasone dipropionate, ...	150605BD	1
Caelo	Betamethasone dipropionate, ...	15412905	1
phönix	Betamethasone dipropionate, ...	15163304	1
Fagron	Betamethasone dipropionate, ...	16C04-B03-320851	1
Fagron	Betamethasone dipropionate, ...	16C04-B03-320852	1
Fagron	Betamethasone dipropionate, ...	1601034-01	1
Caelo	Betamethasone dipropionate, ...	15H28-B06	1
Caelo	Betamethasone dipropionate, ...	15412906	8
Euro OTC	Betamethasone dipropionate, ...	1610014-01	20
Caelo	Betamethasone dipropionate, ...	15412907	4
Fagron	Betamethasone dipropionate, ...	16C04-B03-320850	1
Fagron	Betamethasone dipropionate, ...	2109DM0B0011322	1
Fargon	Betamethasone dipropionate, ...	16C04-B033-24513	1
Caelo	Betamethasone dipropionate, ...	15412909	1
Caelo	Betamethasone dipropionate, ...	15412910	6
Fagron	Betamethasone dipropionate, ...	14C03-B06	1
Gehe	Betamethasone dipropionate, ...	15238701	1
Euro OTC	Betamethasone dipropionate, ...	17B16-B04-332218	1
Noweda	Betamethasone dipropionate, ...	BDP014/1115	1
Caelo	Betamethasone dipropionate, ...	15412916	1
GEHE	Betamethasone dipropionate, ...	15412914	1
Fagron	Betamethasone dipropionate, ...	17B16-B04-332224	2
Fagron	Betamethasone dipropionate, ...	17816B04332224	1
Euro OTC	Betamethasone dipropionate, ...	1610014-015308	1
Caelo	Betamethasone dipropionate, ...	3170717	1
Fagron	Betamethasone dipropionate, ...	17E22-B06-335244	3
Caelo	Betamethasone dipropionate, ...	15H28-B06-313088	1
Sanacorp WE: 12.08.17 ...	Betamethasone dipropionate, ...	15238701	1
Caelo	Betamethasone dipropionate, ...	15412914	2
Fagron	Betamethasone dipropionate, ...	17b16b04332218	1
Caelo	Betamethasone dipropionate, ...	17105903	1
Fagron	Betamethasone dipropionate, ...	17B16-B04	1
Caelo	Betamethasone dipropionate, ...	17105901	8
Sanacorp	Betamethasone dipropionate, ...	1610014-01	1
Fagron	Betamethasone dipropionate, ...	20171127Ma5	1
Sanacorp	Betamethasone dipropionate, ...	1705020-01	1
Fagron	Betamethasone dipropionate, ...	BDP101/0417	1
Klosterring	Betamethasone dipropionate, ...	17B16-B04-332219	2
Caelo	Betamethasone dipropionate, ...	1705020-01	1
Caelo	Betamethasone dipropionate, ...	17105902	4
Sanacorp	Betamethasone dipropionate, ...	17B16-B04-332217	2
Caelo	Betamethasone dipropionate, ...	17105906	3
Fagron	Betamethasone dipropionate, ...	17E22B06336993	1
Euro OTC	Betamethasone dipropionate, ...	1705020-01	9
Caelo	Betamethasone dipropionate, ...	17B16-B04-332220	1
Caelo	Betamethasone dipropionate, ...	17105907	3
Sanacorp	Betamethasone dipropionate, ...	170502001	1

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Supplier	Substance	Batch	Spectra
Fagron	Betamethasone dipropionate, ...	17B16-B04-332219-201	1
Fagron	Betamethasone dipropionate, ...	17H16-B04-340537	1
Fagron	Betamethasone dipropionate, ...	17B16-B04-332217	1
Caelo	Betamethasone dipropionate, ...	17105905	3
Sanacorp	Betamethasone dipropionate, ...	17105911	1
euro//Noweda	Betamethasone dipropionate, ...	1705030-01	1
Caelo	Betamethasone dipropionate, ...	13023002NP	1
Caelo	Betamethasone dipropionate, ...	17105909	2
Gehe	Betamethasone dipropionate, ...	1705020-01	1
Fagron	Betamethasone dipropionate, ...	17E22-B06-336705	1
Fagron	Betamethasone dipropionate, ...	18B06-B05-346218	2
Caelo	Betamethasone dipropionate, ...	17353601	6
Caelo	Betamethasone dipropionate, ...	17353601	1
Delta	Betamethasone dipropionate, ...	18B06-B05-346219	1
Sanacorp	Betamethasone dipropionate, ...	18B06-B05-346218	1
AHD	Betamethasone dipropionate, ...	18B06-B05-346219	1
euro AHD	Betamethasone dipropionate, ...	1801045-015715	1
Caesar & Loretz GmbH	Betamethasone dipropionate, ...	17105902	1
Euro OTC	Betamethasone dipropionate, ...	1801045-01	2
Caelo	Betamethasone dipropionate, ...	17353603	4
Caelo	Betamethasone dipropionate, ...	18090603	4
Caelo	Betamethasone dipropionate, ...	18090602	1
Fagron	Betamethasone dipropionate, ...	18B06-B05-350473	1
euro AHD	Betamethasone dipropionate, ...	1801045-015787	1
Fagron	Betamethasone dipropionate, ...	18B06B0534996	1
Caelo	Betamethasone dipropionate, ...	17105911	1
Caelo	Betamethasone dipropionate, ...	1801045-01	1
Kehr	Betamethasone dipropionate, ...	1705020-01	1
Caelo	Betamethasone dipropionate, ...	18090607	1
Fagron	Betamethasone dipropionate, ...	17E22-B06-336993	1
Sanacorp	Betamethasone dipropionate, ...	BDP102/0817	1
Caelo	Betamethasone dipropionate, ...	18090606	1
Sanacorp	Betamethasone dipropionate, ...	18090607	1

- 78 472 spectra from 565 *Apo-Ident* customers from a total of 25 998 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	400	0	74 096
Type B	0	687	0	126 205
Type C	0	453	4	78 472

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 99.1266 %)
Type C	100.0000 % (> 99.8817 %)	99.1247 % (> 98.4683 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20930	20930	0.00	16.34
21366	21250	1.45	17.31
21250	21250	0.00	17.57
22372	22372	0.00	15.74
21716	21716	0.00	15.39
22898	20930	2.57	18.10

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Betamethasone valerate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20026-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Betamethasone valerate; Betamethasoni valeras

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Betamethasone valerate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Betamethasone va...	12K07-N23	20887	40	20121119
Euro OTC	Betamethasone va...	1208014-01	20920	40	20120928
Caelo	Betamethasone va...	13091213	21215	40	20130506
Fagron	Betamethasone va...	13K29-B32-288243	21566	40	20131210
Caelo	Betamethasone va...	13225507	21588	34	1706018

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Betamethasone va...	1406019-01	21645	40	20140725
Fagron	Betamethasone va...	13K05-B08-292651	21674	40	1511154
Euro OTC	Betamethasone va...	1510037	22249	40	20151215*
Euro OTC	Betamethasone va...	1610010	22861	40	20161116*
Euro OTC	Betamethasone va...	1811008	24349	40	20181207*
Euro OTC	Betamethasone va...	1510037	22249SI	20	20151215*
Euro OTC	Betamethasone va...	1811008	24349SI	30	20181207*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 444 spectra of 12 reference samples from the substance/substance group *Betamethasone valerate*. These samples are listed above in the [calibration samples](#) section.
- 74052 spectra from a total of 1613 batches from further 372 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 [†].

- 489 spectra of 17 reference samples from the substance/substance group *Betamethasone valerate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Betamethasone valerate	13K29-B32-288243	21566 [†]	20
Caelo	Betamethasone valerate	13225507	21588 [†]	26
Euro OTC	Betamethasone valerate	1406019-01	21645 [†]	20
Fagron	Betamethasone valerate	13K05-B08-292651	21674 [†]	20
Euro OTC	Betamethasone valerate	1510037	22249 [†]	20
Euro OTC	Betamethasone valerate	1606023	22716	40
Caelo	Betamethasone valerate	170787	23332	40
Euro OTC	Betamethasone valerate	1704019	23396	40
Caelo	Betamethasone valerate	172716	23683	40
Euro OTC	Betamethasone valerate	1801024	23967	40
Euro OTC	Betamethasone valerate	1510037	22249SI [†]	10

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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	Betamethasone valerate	1606023	22716SI	34
Euro OTC	Betamethasone valerate	1610010	22861SI	30
Caelo	Betamethasone valerate	170787	23332SI	20
Euro OTC	Betamethasone valerate	1704019	23396SI	29
Caelo	Betamethasone valerate	172716	23683SI	20
Euro OTC	Betamethasone valerate	1801024	23967SI	40

- 126 403 spectra from a total of 2778 batches from further 781 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.

- 1651 spectra from 444 *Apo-Ident* customers from 387 batches from the substance/substance group *Betamethasone valerate*.

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	11K18-N09	2
Caelo	Betamethasone valerate	10296705	2
Euro OTC	Betamethasone valerate	1108045-01	2
Fagron	Betamethasone valerate	NP1351M	1
Fagron	Betamethasone valerate	12B28-N01	8
Caelo	Betamethasone valerate	11131917	2
Euro OTC	Betamethasone valerate	1108045-02	3
Caelo	Betamethasone valerate	12003403	7
Hepart AG, CH-8280 Kreu...	Betamethasone valerate	11131914	2
Caelo	Betamethasone valerate	11131909	1
Caelo	Betamethasone valerate	1108045-03	4
Caesar & Loretz GmbH, 4...	Betamethasone valerate	10296707	1
agron/Krieger	Betamethasone valerate	12B2B-N01	1
Euro OTC	Betamethasone valerate	2507211181	1
Gehe	Betamethasone valerate	12003403	1
Caelo	Betamethasone valerate	1131914	1
Euro OTC	Betamethasone valerate	1108045-03	6
Caelo	Betamethasone valerate	12003406	6
Fiebig ek: 45,65EUR	Betamethasone valerate	12B28-N01	1
Noweda	Betamethasone valerate	11131902	1
Caelo	Betamethasone valerate	12003405	8
Fagron	Betamethasone valerate	12G09-N07	22
Caelo	Betamethasone valerate	12B28-N01	1
Noweda	Betamethasone valerate	12G09-N07	1
Caelo	Betamethasone valerate	12003402	1
Euro OTC	Betamethasone valerate	110804-02	1
Caesar & Loretz GmbH	Betamethasone valerate	11131917	1
Fagron	Betamethasone valerate	612211181	1
Noweda	Betamethasone valerate	11B21-N02	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	Betamethasone valerate	18121206	1
Fagron	Betamethasone valerate	20101012-1	1
Caelo	Betamethasone valerate	11131914	1
Caelo	Betamethasone valerate	12G09-N07	3
Sanacorp	Betamethasone valerate	12G09-N07	1
Caelo	Betamethasone valerate	12003410	1
Caelo	Betamethasone valerate	12003407	1
Caelo	Betamethasone valerate	12003411	3
Fagron	Betamethasone valerate	12K07-N23	6
Fagron	Betamethasone valerate	11A04-N02	1
Caelo	Betamethasone valerate	12229802	3
Gehe	Betamethasone valerate	12003409	1
Euro OTC	Betamethasone valerate	1208014-01	11
Caelo	Betamethasone valerate	1208014-01	1
Caelo	Betamethasone valerate	12g09-n07	1
Fagron	Betamethasone valerate	12L11-N01	17
Caelo	Betamethasone valerate	12K07-N23	1
Eigenherstellung	Betamethasone valerate	9070313	1
Caelo	Betamethasone valerate	1113	1
Fagron	Betamethasone valerate	2B28-N01	1
Caelo	Betamethasone valerate	10296701	1
Phönix	Betamethasone valerate	12229807	1
Caelo	Betamethasone valerate	12229805	9
Caelo	Betamethasone valerate	12229809	2
vdl	Betamethasone valerate	12003411	1
Holdermann	Betamethasone valerate	1208014-01	1
Phoenix	Betamethasone valerate	12003409	2
Caelo	Betamethasone valerate	12229804	3
Fagron	Betamethasone valerate	13D03-N07	35
Caelo	Betamethasone valerate	12229806	5
Euro OTC	Betamethasone valerate	1208014-02	11
Anzag	Betamethasone valerate	12L11-N01	1
Caelo	Betamethasone valerate	12229808	12
Caesar/Lorenz	Betamethasone valerate	12003403	1
Euro OTC	Betamethasone valerate	13D03-N07	1
Caelo	Betamethasone valerate	12003409	1
Caelo	Betamethasone valerate	13091201	2
Caelo	Betamethasone valerate	12229812	9
Euro OTC	Betamethasone valerate	120812-02	1
Holdermann	Betamethasone valerate	120801402	1
Caelo	Betamethasone valerate	12229810	3
EuRho	Betamethasone valerate	1208014-02	1
Fagron	Betamethasone valerate	13d03-n07	3
Bombastus	Betamethasone valerate	12L11-N01	1
Caelo	Betamethasone valerate	13D03-N07	2
Caelo	Betamethasone valerate	12229811	6
Fiebig 27.06.13 EK47,81	Betamethasone valerate	B9/131	1
AHC 01.07.13 EK 48,05	Betamethasone valerate	12K07-N23	1
Noweda	Betamethasone valerate	1208014-02	2
Caelo	Betamethasone valerate	12229813	2
Phönix	Betamethasone valerate	13091201	2
Phönix	Betamethasone valerate	13D03-N07	1
Caelo	Betamethasone valerate	11131905	1
Noweda	Betamethasone valerate	12229832	1
Fagron	Betamethasone valerate	NS0706M	3
Euro OTC	Betamethasone valerate	120801402	2
Fagron	Betamethasone valerate	NS2072M	1
Euro OTC	Betamethasone valerate	3313U-01181	1
Caelo	Betamethasone valerate	13091203	10
Fagron	Betamethasone valerate	13G19-N01	46

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Supplier	Substance	Batch	Spectra
Euro OTC	Betamethasone valerate	12L11-N01	1
Caelo	Betamethasone valerate	2x12229813	1
Euro OTC	Betamethasone valerate	110804503	1
A.H.D.	Betamethasone valerate	13D03-N07	1
Euro OTC	Betamethasone valerate	1208014-03	4
Alliance healthcare	Betamethasone valerate	13D03-N07	1
Phönix	Betamethasone valerate	BV-BLT186/0512	1
Caelo	Betamethasone valerate	12L11-N01	1
Caelo	Betamethasone valerate	13091204	4
Caelo	Betamethasone valerate	13091207	7
Caelo	Betamethasone valerate	13091209	4
Europ Ots Pharma	Betamethasone valerate	12111-N01	1
Fagron	Betamethasone valerate	NT0597M	2
Phönix	Betamethasone valerate	13091209	2
Fagron	Betamethasone valerate	120801402	1
Oberlinden- Apotheke	Betamethasone valerate	C0073/1	3
Caelo	Betamethasone valerate	210112	1
Caelo	Betamethasone valerate	1208014-03	1
Phönix Gotha	Betamethasone valerate	12229808	1
Caelo	Betamethasone valerate	13G19-N01	1
Noweda	Betamethasone valerate	1208014-01	1
Symbiotica Spec.	Betamethasone valerate	1208014-04	1
Gehe	Betamethasone valerate	1208014-04	1
Caelo	Betamethasone valerate	13091212	6
Fagron	Betamethasone valerate	13g19-n01	2
Euro OTC	Betamethasone valerate	1208014-04	4
Fagron	Betamethasone valerate	13G19N01	1
Phönix	Betamethasone valerate	13091212	2
Caelo	Betamethasone valerate	13091206	1
Caelo	Betamethasone valerate	B03041205	1
Fagron	Betamethasone valerate	13G19-N01	1
Gehe am 03.02.2014	Betamethasone valerate	13091210	3
Caelo	Betamethasone valerate	13091213	6
Alliance Health 06.02.2. . .	Betamethasone valerate	13091207	1
Euro OTC	Betamethasone valerate	120801403	1
Euro OTC	Betamethasone valerate	120801404	1
Sanacorp	Betamethasone valerate	13091210	1
Noweda	Betamethasone valerate	13091203	1
Fagron	Betamethasone valerate	11E18-N03	2
Caelo	Betamethasone valerate	13091210	3
Caelo	Betamethasone valerate	13091205	11
Hirsch	Betamethasone valerate	13G19-No1	1
Fargon/Anzag	Betamethasone valerate	13G19-N01	1
Caelo	Betamethasone valerate	13225503	4
Gehe	Betamethasone valerate	13091211	1
noweda	Betamethasone valerate	1208014-04	1
Euro OTC	Betamethasone valerate	1311039-01	19
Fagron	Betamethasone valerate	12L11-N01	1
Fagron	Betamethasone valerate	13K29-B32-288246	5
Caesar & Loretz GmbH Hi. . .	Betamethasone valerate	120801402	1
Fagron	Betamethasone valerate	13K29-B32	5
Fagron	Betamethasone valerate	NT059M	1
Fagron	Betamethasone valerate	13K29-B32-288250	3
Caelo	Betamethasone valerate	13091211	3
Fagron	Betamethasone valerate	13K29B32	1
Euro OTC	Betamethasone valerate	2014Q1181	1
Fagron	Betamethasone valerate	13K29-B32-288247	14
Sanacorp	Betamethasone valerate		1
Noweda	Betamethasone valerate	13091205	1
Euro OTC	Betamethasone valerate	131103901	1

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Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	13K29-B32-288244	2
Phonix	Betamethasone valerate	13K29-B32	1
Caelo	Betamethasone valerate	13225505	8
	Betamethasone valerate	1208014-04	1
Caelo	Betamethasone valerate	18071403	1
Euro OTC	Betamethasone valerate	1311039	1
Caelo	Betamethasone valerate	13225504	5
Caelo	Betamethasone valerate	13225508	9
Fagron	Betamethasone valerate	13K29-B12-288247	1
Fagron	Betamethasone valerate	13K29-B32-28824	1
Noveda	Betamethasone valerate	1311039-01	1
Caelo	Betamethasone valerate	10296707	1
Ichthyol-Gesellschaft	Betamethasone valerate	13k29-B32-288247	1
Fagron	Betamethasone valerate	13K29B32288243	1
Fagron	Betamethasone valerate	14C19-B02-292653	6
Caelo	Betamethasone valerate	13225515	7
Caelo	Betamethasone valerate	13225502	2
GEHE 17.06.2014	Betamethasone valerate	13225503	1
Fagron	Betamethasone valerate	1311039-01	1
Euro OTC	Betamethasone valerate	131139-01	1
Euro OTC	Betamethasone valerate	1406019-01	21
NEWCHEM	Betamethasone valerate	1311039-01	1
Caelo	Betamethasone valerate	13225507	2
Fagron	Betamethasone valerate	13K29-B32-288248	3
Gehe	Betamethasone valerate	1712E-01181	1
Caelo	Betamethasone valerate	14188603	5
Phoenix Goettin	Betamethasone valerate	13225508	1
Fagron	Betamethasone valerate	14C19-B02-292648	1
Phönix Gotha	Betamethasone valerate	13091213	1
Fagron	Betamethasone valerate	13K29-B23-288246	1
Caelo	Betamethasone valerate	13225509	2
Caelo	Betamethasone valerate	14188602	2
Fagron	Betamethasone valerate	292652	1
Fargon/Alliance HC	Betamethasone valerate	13K29-B32-288247	1
AHD 17.11.14 EK 18,11	Betamethasone valerate	13091205	1
Caelo	Betamethasone valerate	13225607	1
Caelo	Betamethasone valerate	13K29-B32-288247	1
Caelo	Betamethasone valerate	14188604	6
Caelo	Betamethasone valerate	13225516	9
Fagron	Betamethasone valerate	13117-B08-292649	2
Caelo	Betamethasone valerate	1406019-01	1
Symbiotica Spec.	Betamethasone valerate	1406019-01	3
Fagron	Betamethasone valerate	13/17-B08-292649	2
Caelo	Betamethasone valerate	13012015C	1
Fagron	Betamethasone valerate	14C19-B02-296169	1
Fagron	Betamethasone valerate	14C19-B02	3
Caelo	Betamethasone valerate	NT0597M	1
Fagron	Betamethasone valerate	14c19-b02-292650	1
Fagron	Betamethasone valerate	14C19-B02-292646	1
Caelo	Betamethasone valerate	14C19-B02-292653	1
Euro OTC	Betamethasone valerate	140601901	1
Phönix Gotha	Betamethasone valerate	14188608	1
Caelo	Betamethasone valerate	14188608	6
Fagron	Betamethasone valerate	13K05-B08-292652	1
AHDE / Cael 17.02.2015	Betamethasone valerate	13225516	1
Caelo	Betamethasone valerate	13K05B08292652	1
Euro OTC	Betamethasone valerate	14C19-B02-292650	2
Fagron	Betamethasone valerate	13K29-B32-288245	1
Fagron	Betamethasone valerate	14C19-B02-292650	3
Euro OTC	Betamethasone valerate	1206014-02	1

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Supplier	Substance	Batch	Spectra
Caelo	Betamethasone valerate	14188609	5
noweda	Betamethasone valerate	1406019-01	1
Fagron	Betamethasone valerate	14C19-B02-296168	4
Caesar & Loretz GmbH	Betamethasone valerate	13225504	1
Fagron	Betamethasone valerate	13k29b32288247	1
Fagron	Betamethasone valerate	13K05-B08	1
Fagron	Betamethasone valerate	14G30B05296172	1
Fagron	Betamethasone valerate	13K05-B08-292647	2
Euro OTC	Betamethasone valerate	1406019-02	23
AHD	Betamethasone valerate	1406019-02	2
Fagron	Betamethasone valerate	14G30-B05-296172	3
Caelo	Betamethasone valerate	14188619	2
Fagron	Betamethasone valerate	13K05-B08-291663	1
Fagron	Betamethasone valerate	13k29-b32-289364	1
Fagron	Betamethasone valerate	BV019/0514	3
Caelo	Betamethasone valerate	15075802	18
Fagron	Betamethasone valerate	14188603	1
Fagron	Betamethasone valerate	14G30-B05-296173	11
Caelo	Betamethasone valerate	14188610	6
Allianz Healthcare 27.0...	Betamethasone valerate	15075802	1
Fagron	Betamethasone valerate	14G30-B05-296175	2
Caesar&Loretz GmbH/Anzag	Betamethasone valerate	15075802	1
Fagron	Betamethasone valerate	14C19B02	1
Euro OTC	Betamethasone valerate	140601902	1
Caelo	Betamethasone valerate	1406019-02	1
Euro OTC	Betamethasone valerate	13K29-B32-289364	1
Caelo	Betamethasone valerate	14188617	2
Fagron	Betamethasone valerate	14G30-B05-296172	1
Fagron	Betamethasone valerate	14H28-B01	3
Sanacorp	Betamethasone valerate	14188602	1
Fagron	Betamethasone valerate	14H28-B01-302865	12
Fagron	Betamethasone valerate	14G30-B05	3
Caelo	Betamethasone valerate	15075803	7
Fagron	Betamethasone valerate	15B24-B04-307015	3
Caelo	Betamethasone valerate	14H28-B01-302865	1
Euro OTC	Betamethasone valerate	1406019-03	25
Fagron	Betamethasone valerate	14H28-B01-302683	1
Oberlinden Apotheke	Betamethasone valerate	C0073/115040	3
Caelo	Betamethasone valerate	1488610	1
Fagron	Betamethasone valerate	14G30-B05-309520	6
Fagron	Betamethasone valerate	14G30B05309519	1
Fagron	Betamethasone valerate	14H28B01	1
Fagron	Betamethasone valerate	14G30-B05-309519	1
Euro OTC	Betamethasone valerate	140601903	2
Fagron	Betamethasone valerate	BV-BLT225/0514	1
Caelo/Sanacorp	Betamethasone valerate	15075803	1
Caelo	Betamethasone valerate	1406019-03	2
Fagron	Betamethasone valerate	14G30-B05-309518	2
Gehe	Betamethasone valerate	14H28-B01-302863	1
Gehe	Betamethasone valerate	14H25-B01-302863	1
Fagron	Betamethasone valerate	14G30-B05-29617	1
Fagron	Betamethasone valerate	14H28-B01-302866	3
Fagron	Betamethasone valerate	14c19-b02-296169	1
Fagron	Betamethasone valerate	12K07N23	1
Fagron	Betamethasone valerate	14H28-B01-302863	4
caesar&loretz,phönix	Betamethasone valerate	14188606	1
Caelo	Betamethasone valerate	BV-BLT225/0514	1
Fagron	Betamethasone valerate	309520	1
Caelo	Betamethasone valerate	15075805	6
Euro	Betamethasone valerate	1406019-03	3

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Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	15B24-B04-307016	12
Caelo	Betamethasone valerate	15075804	7
Fragron	Betamethasone valerate	BV-BLT225/0514	2
Fagron	Betamethasone valerate	14h28-b01-302865	2
Caelo	Betamethasone valerate	15262603	11
Fagron	Betamethasone valerate	14G30-B05-309521	1
Caesar und Loretz	Betamethasone valerate	15075803	1
Euroo	Betamethasone valerate	1406019-03	1
Fagron	Betamethasone valerate	14H28-B01-302864	5
Fagron	Betamethasone valerate	14H28-B01-302877	3
Caelo	Betamethasone valerate	15075810	6
Noweda/Ceasar Lorenz	Betamethasone valerate	14188606	1
Euro OTC	Betamethasone valerate	1406011903	1
Bombastus	Betamethasone valerate	1510037-01	1
Caelo	Betamethasone valerate	15262602	2
Fagron	Betamethasone valerate	15F16-B04-314054	2
Euro OTC	Betamethasone valerate	1510037-01	17
Noweda	Betamethasone valerate	15075812	1
Caelo	Betamethasone valerate	1510037-01	2
Caelo	Betamethasone valerate	140601903	1
Caelo	Betamethasone valerate	15262604	9
Cael Sanacorp 05.02.2016	Betamethasone valerate	14H28-B01-302864	1
Fagron	Betamethasone valerate	15824-B04	1
Caelo	Betamethasone valerate	15075809	2
Fagron	Betamethasone valerate	15F16-B04-314054/201	1
Fagron	Betamethasone valerate	14H28-B01-302864/201	1
Caelo	Betamethasone valerate	150758036	1
Caelo	Betamethasone valerate	1526604	1
AHD/Fargon	Betamethasone valerate	14H28-B01-302865	1
Caelo	Betamethasone valerate	15262607	6
Noweda	Betamethasone valerate	14H28B01302863	1
Noweda	Betamethasone valerate	1406019-03	2
Caelo	Betamethasone valerate	14G30-B05	1
Caelo	Betamethasone valerate	15075812	3
Fagron	Betamethasone valerate	1406019-03	1
Fagron	Betamethasone valerate	14H28B01302864	1
Hedinger	Betamethasone valerate	14H28-B01-302877	1
Caelo	Betamethasone valerate	15B24-B04-307016	1
Fagron	Betamethasone valerate	15f16-b04314054	1
Caelo	Betamethasone valerate	123345	1
Caleo/Phönix	Betamethasone valerate	1522609	1
Fagron	Betamethasone valerate	15I16-B07-317416	1
Fagron	Betamethasone valerate	14H28-B01-305470	1
Oberlinden Apotheke	Betamethasone valerate	c073/115040	1
Fagron	Betamethasone valerate	15/16-B07-317428	3
Fagron	Betamethasone valerate	90616-2	1
Fagron	Betamethasone valerate	15F16-B04-315328	3
Fagron	Betamethasone valerate	15B24-B04	1
Fagron	Betamethasone valerate	15/16-B07-317416	3
AHD 15.06.16 EK:18,44	Betamethasone valerate	15398505	1
Caelo	Betamethasone valerate	15262609	3
Symbiotica	Betamethasone valerate	14H28B01302863	1
Fagron	Betamethasone valerate	15F16-B04	2
Caelo	Betamethasone valerate	15398501	12
Caelo	Betamethasone valerate	15262606	4
Ebert u. Jacobi 16.0...	Betamethasone valerate	15/16-B07-317417	1
Fagron	Betamethasone valerate	15I16-B07	1
Caelo	Betamethasone valerate	1526213	1
Caelo	Betamethasone valerate	15398505	11
Caelo	Betamethasone valerate	15/16-B07-319228	2

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Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	15/16-B07-319228	3
Phönix WE:16.07.2016 ...	Betamethasone valerate	1510037-01	1
Fagron	Betamethasone valerate	16B18-B02-320971	5
Caelo	Betamethasone valerate	15B24-B04	1
Euro/Alliance Healthcare	Betamethasone valerate	1510037-01	1
Caelo	Betamethasone valerate	1516-B07-319228	1
Fargon/Anzag	Betamethasone valerate	16B18-B02-320971	1
Fargon/Alliance HC	Betamethasone valerate	16B18-B02-322111	1
Caelo	Betamethasone valerate	15398506	23
Fagron	Betamethasone valerate	15I16-B07-319228	2
Fagron	Betamethasone valerate	700103-0004	1
Euro OTC	Betamethasone valerate	1606023-01	29
Symbiotica/ Anzag	Betamethasone valerate	1606023-01	2
Euro OTC	Betamethasone valerate	15398501	1
Fagron	Betamethasone valerate	B07-317416	1
AHL	Betamethasone valerate	15398501	1
Caelo	Betamethasone valerate	160216BV	1
Fagron	Betamethasone valerate	15I16-B07-319832	2
Symbiotica Spec/Noweda	Betamethasone valerate	1208014-04	1
phönix	Betamethasone valerate	15/16B07-319228	1
Euro OTC	Betamethasone valerate	15/16-B07-319228	1
Caelo	Betamethasone valerate	16B18-B02-320971	1
Caelo	Betamethasone valerate	1538506	1
Caelo	Betamethasone valerate	15398515	17
Caelo	Betamethasone valerate	161125BV/15398512	1
Caelo	Betamethasone valerate	1606023-01	4
Fagron	Betamethasone valerate	BV036/1215	1
Caelo	Betamethasone valerate	15075811	1
Fagron	Betamethasone valerate	16B18-B02-322111	1
Fagron	Betamethasone valerate	15/16-B07-319832	1
Gehe	Betamethasone valerate	15398501	1
Fagron	Betamethasone valerate	16E23-B03-324800	5
Caelo	Betamethasone valerate	15398512	13
Caelo	Betamethasone valerate	15262612	1
Caelo	Betamethasone valerate	15398503	2
ALH	Betamethasone valerate	15398512	1
Fagron	Betamethasone valerate	16B18B02320971	1
Fagron	Betamethasone valerate	16E23-B03-324799	6
Fagron	Betamethasone valerate	16e23b03324800	1
Euro OTC	Betamethasone valerate	16100100-01	1
Caelo	Betamethasone valerate	1610010-01	4
Caelo	Betamethasone valerate	15L21-B03-318663	1
Fagron	Betamethasone valerate	15I16-B07-319832	2
Euro OTC	Betamethasone valerate	1610010-01	31
Fagron	Betamethasone valerate	16B18-B02	4
Caelo	Betamethasone valerate	16270501	10
Caelo	Betamethasone valerate	15F16-B04-315327	1
Alliance Healthcare	Betamethasone valerate	1610010-01	1
Caelo	Betamethasone valerate	1627051	1
Fagron	Betamethasone valerate	16b18-b02-324798	1
Caelo	Betamethasone valerate	15398504	2
phönix	Betamethasone valerate	15398515	1
Euro OTC	Betamethasone valerate	160623-01	1
Fagron	Betamethasone valerate	16e23-b03-324800	1
Fagron	Betamethasone valerate	15398515	1
Caelo	Betamethasone valerate	16B18-B02-322121	2
Fagron	Betamethasone valerate	16B18-B02-323034	2
Caelo	Betamethasone valerate	14188605	1
Fagron	Betamethasone valerate	16B18-B02-324798	2
Caelo	Betamethasone valerate	16E23-B03	1

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Supplier	Substance	Batch	Spectra
Caelo	Betamethasone valerate	15262610	3
GEHE	Betamethasone valerate	16270501	1
Fagron	Betamethasone valerate	15116-B07	1
Caelo	Betamethasone valerate	15398514	1
Fagron	Betamethasone valerate	16B18-B02-323033	1
Fagron	Betamethasone valerate	16E23-B03	6
Caelo	Betamethasone valerate	16270503	7
Caelo	Betamethasone valerate	16E23-B03-324799	2
Fagron	Betamethasone valerate	16818-B02-323033	1
Fagron	Betamethasone valerate	16B18-B02-322121	2
Caelo	Betamethasone valerate	15398513	3
Fagron	Betamethasone valerate	16B18-B02320971	1
Fagron	Betamethasone valerate	15F16-B04-314055	1
Fagron	Betamethasone valerate	1516-B07-317416	1
Fagron	Betamethasone valerate	16818-B02-320971	1
Euro OTC	Betamethasone valerate	16270505	1
Caelo	Betamethasone valerate	16270502	22
Fagron	Betamethasone valerate	16E23-B03-328128	8
Caelo	Betamethasone valerate	16270505	8
Fagron	Betamethasone valerate	16E23-B03-327354	3
Caelo	Betamethasone valerate	16270504	1
Symbiotica	Betamethasone valerate	1610010-01	2
Gehe	Betamethasone valerate	16270505	1
Fagron	Betamethasone valerate	16B18-B02-322109	4
Fagron	Betamethasone valerate	15I16-Bo7-319832	1
Fagron	Betamethasone valerate	16E23B03328128	1
Fagron	Betamethasone valerate	7890	1
Caelo	Betamethasone valerate	16270509	3
Caelo	Betamethasone valerate	16270511	13
Euro OTC	Betamethasone valerate	16E23-B03-328128	2
Fagron	Betamethasone valerate	15/16-B07	1
Noweda/ Infecto Pharm	Betamethasone valerate	16270505	1
Cealo/Noweda	Betamethasone valerate	16270509	2
Fagron	Betamethasone valerate	16H22-B06-329231	3
Caelo	Betamethasone valerate	16270513	8
Caesar&Loretz GmbH,PHön...	Betamethasone valerate	16270509	1
Fagron	Betamethasone valerate	16270513	1
Fagron	Betamethasone valerate	16H22-B06	2
Euro OTC	Betamethasone valerate	1704019-01	47
Fagron	Betamethasone valerate	16H22B06330524	2
AHD	Betamethasone valerate	15398515	1
EuRho / Phoenix	Betamethasone valerate	1704019-01	1
Caelo	Betamethasone valerate	16720513	1
Caelo	Betamethasone valerate	15F16-B04-314054	1
EurRho/Gehe	Betamethasone valerate	1610010-01	1
Fagron	Betamethasone valerate	16H22-B06-329223	1
Fagron	Betamethasone valerate	BV008/045	1
Euro/direkt	Betamethasone valerate	1704019-01	1
Caelo	Betamethasone valerate	16270514	2
Caelo	Betamethasone valerate	17078703	12
phönix	Betamethasone valerate	16e23-b03-327350	1
Fagron	Betamethasone valerate	16H22-B06-330523	2
Caelo	Betamethasone valerate	170401901	2
Finteler Apotheke	Betamethasone valerate	17C29-B04-333688	2
Caelo	Betamethasone valerate	17078702	1
Caelo	Betamethasone valerate	1708701	1
Fagron	Betamethasone valerate	16H22-B06-330524	2
/Sanacorp	Betamethasone valerate	17078701	1
Caelo	Betamethasone valerate	17078103	1
EuRho	Betamethasone valerate	1208014-01	1

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Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	1704019-01	3
Euro OTC	Betamethasone valerate	1704019-01	1
Caelo	Betamethasone valerate	17078701	9
Fagron	Betamethasone valerate	16E23-B03-327350	3
Bombastus	Betamethasone valerate	1704019-01	2
Fagron	Betamethasone valerate	17C29-B04-334329	3
Caelo	Betamethasone valerate	17/251/Bv	1
Fagron, Noweda 07.11.2017	Betamethasone valerate	16H22-B06-329223	1
Caelo	Betamethasone valerate	17078704	3
Fagron	Betamethasone valerate	17C29-B04-335676	5
Caelo	Betamethasone valerate	17078705	1
Fagron	Betamethasone valerate	17C29-B04-335657	5
GEHE	Betamethasone valerate	17078701	2
Caesar & Loretz GmbH	Betamethasone valerate	17078701	1
Fagron	Betamethasone valerate	17C29-335654	1
Caelo	Betamethasone valerate	17078711	1
Euro OTC	Betamethasone valerate	1704019	1
Caelo	Betamethasone valerate	17078712	6
Caelo	Betamethasone valerate	17078713	9
Caelo	Betamethasone valerate	17C29-B04	2
Caelo	Betamethasone valerate	16H22-B06-331273	1
Caelo	Betamethasone valerate	1704019-01	2
Fagron	Betamethasone valerate	16E23-B03-3247990855	1
Caelo	Betamethasone valerate	17078714	6
Fagron	Betamethasone valerate	16H22-B06-330522	1
Caelo	Betamethasone valerate	17078719	8
Fagron	Betamethasone valerate	17C29-B04-335658	1
Caelo	Betamethasone valerate	17078716	1
Sanacorp W.E: 18.01.18 ...	Betamethasone valerate	1704019-01	1
Jenne	Betamethasone valerate	17078712	1
Fagron	Betamethasone valerate	17G31-B04-338575	2
AHD	Betamethasone valerate	17078714	1
Euro/Gehe	Betamethasone valerate	1704019-01	1
Fagron	Betamethasone valerate	17G31B04338575	1
Fagron	Betamethasone valerate	14G31-B04-342639	1
Caelo	Betamethasone valerate	1707814	1
Caelo	Betamethasone valerate	17078720	4
Noweda	Betamethasone valerate	BV01090117	1
Caelo	Betamethasone valerate	17078715	8
Euro OTC	Betamethasone valerate	1801024-01	15
Fagron	Betamethasone valerate	17G31-B04-341576-201	1
Caelo	Betamethasone valerate	17271603	10
Fagron	Betamethasone valerate	17C29B043356575581	1
Farmabios S. p. A./ Now...	Betamethasone valerate	17078715	1
Fagron	Betamethasone valerate	17C29-B04-335654	2
Ichthyol-Gesellschaft	Betamethasone valerate	17078720	1
Fagron	Betamethasone valerate	17G31-B04-341576	3
Fagron	Betamethasone valerate	17c29-b04-335657	2
Fagron	Betamethasone valerate	17G31-B04	2
Caelo	Betamethasone valerate	17271601	3
Fagron	Betamethasone valerate	17G31-B04-3415765	1
Caelo	Betamethasone valerate	17271602	1
Fagron	Betamethasone valerate	17G31-B04-342639	1
Sanacorp	Betamethasone valerate	17078715	1
Caelo	Betamethasone valerate	17329001	4
GEHE	Betamethasone valerate	17078720	1
Caelo	Betamethasone valerate	1707815	1
Fagron	Betamethasone valerate	BV-BLT250/0616	1
Fagron	Betamethasone valerate	17G31-B04-339785	1
Fagron	Betamethasone valerate	17K16-B08-345555	2

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Supplier	Substance	Batch	Spectra
Euro OTC	Betamethasone valerate	1704019-0	1
Fagron	Betamethasone valerate	17G31-B04-339784	2
Fagron	Betamethasone valerate	17K16-B08-345541	3
Fagron	Betamethasone valerate	BV106/0717	1
Caelo	Betamethasone valerate	17271604	1
Caelo	Betamethasone valerate	17K16-B08-345541	1
Fagron	Betamethasone valerate	17271604	2
Fagron	Betamethasone valerate	BV009/0117	1
Cealo/Gehe	Betamethasone valerate	1801024-01	1
Fagron	Betamethasone valerate	17K16-B08-348042	2
Caelo	Betamethasone valerate	17329002	7
Caelo	Betamethasone valerate	17K16-B0/8-347310	1
Caelo	Betamethasone valerate	1801024-01	2
Caelo	Betamethasone valerate	17K16-B08-347912	1
Caelo	Betamethasone valerate	17329003	4
Fagron	Betamethasone valerate	17K16-B08-347912	1
Cealo/Gehe	Betamethasone valerate	17329002	1
Cealo/Gehe	Betamethasone valerate	1739002	1
Caelo	Betamethasone valerate	17329008	4
Fagron	Betamethasone valerate	17K16-B08-349774	1
Euro OTC	Betamethasone valerate	1704018-01	1
Fagron	Betamethasone valerate	17K16-B08-347309	1
Fagron	Betamethasone valerate	17K16-B08-349755	3
Fagron	Betamethasone valerate	17K16-B08-345542	1
euro//Noweda	Betamethasone valerate	1801024-01	2
Fagron	Betamethasone valerate	17329016	1
Fagron	Betamethasone valerate	17K16-B08-347309	1
Euro OTC	Betamethasone valerate	1739002	1
Caelo	Betamethasone valerate	17329018	9
Kehr	Betamethasone valerate	1801024-01	1
Fagron	Betamethasone valerate	17K16-B08	1
Caelo	Betamethasone valerate	17329015	1
Fagron	Betamethasone valerate	18G03-B03-351450	1
Caelo	Betamethasone valerate	18199902	2
Fagron	Betamethasone valerate	18G03-B03-352460	1
Caelo	Betamethasone valerate	18199907	2

- 77 278 spectra from 565 *Apo-Ident* customers from a total of 25 755 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	444	0	74 052
Type B	0	489	0	126 403
Type C	0	1635	16	77 278

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.6486 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.7730 %)
Type C	100.0000 % (> 99.8817 %)	99.0309 % (> 98.8492 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21215	22249	4.36	33.30
20920	22861	4.80	35.44
21566	24349	5.48	33.36
21588	21588	0.00	27.55
22249	22249	0.00	29.88
21645	24349	4.28	32.44
20887	24349	8.18	33.28
21674	21674	0.00	27.29
22861	22861	0.00	33.69
24349	24349	0.00	30.52

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Betamethasone, micronized**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20943-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Betamethasone, micronized; Betamethasonum, micronisatum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Betamethasone, micronized*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Betamethasone, m...	12D26-N08	20943	40	1402096
Fagron	Betamethasone, m...	13H08-N06	21579	40	1411037
Fagron	Betamethasone, m...	11H31-B06-288219	22493	40	1608324

Validation samples

A total of 280 317 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 *Betamethasone, micronized*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Betamethasone, micronized*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Betamethasone, micronized	13H08-N06	21579 [†]	20
Fagron	Betamethasone, micronized	14C13-B02-296165	22897	40
Fagron	Betamethasone, micronized	15L09-B05-324091	22904	40

- 126 792 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 26 spectra from 18 *Apo-Ident* customers from 20 batches from the substance/substance group *Betamethasone, micronized*.

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone, micronized	9J26-N08	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
Noweda	Betamethasone, micronized	12B20-N05	1
Fagron	Betamethasone, micronized	11/14-N02	1
Fagron	Betamethasone, micronized	12B20-N05	2
Fagron	Betamethasone, micronized	9071304	1
Caelo	Betamethasone, micronized	11/14-N02	1
Noweda	Betamethasone, micronized	M-X01-120301m1	1
Unisan	Betamethasone, micronized	Retest09K25-N13	1
Fiebig	Betamethasone, micronized	12J01-120301-m1	1
Fagron	Betamethasone, micronized	9K25-N13	1
Fagron	Betamethasone, micronized	12J01-N02	1
Fagron	Betamethasone, micronized	12D26-N08	1
Phönix	Betamethasone, micronized	12B20-N05	1
Fagron	Betamethasone, micronized	11H31-B06-288217	1
Fagron	Betamethasone, micronized	14C13-B02-296164	2
Fagron	Betamethasone, micronized	12D26-N08	1
Fagron	Betamethasone, micronized	14C13-B02-296154	1
Fagron	Betamethasone, micronized	14C13-B02	1
Fagron	Betamethasone, micronized	14C13-B02-305561	1
Fagron	Betamethasone, micronized	14c13-bo2-305561	1
Symbiotec Pharmed Ltd. . .	Betamethasone, micronized	14C13-B02	1
Fagron	Betamethasone, micronized	15L09-B05322119	1
Fagron	Betamethasone, micronized	15L09-B05	1
Fagron	Betamethasone, micronized	16I07-B01-341871	1

- 78 903 spectra from 565 *Apo-Ident* customers from a total of 26 117 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Betamethasone, micronized* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Betamethasone, micronized* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	13	13	78 903

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	50.0000 % (> 38.4615 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22493	22493	0.00	20.97
21579	21579	0.00	22.06
20943	20943	0.00	18.01

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Bifonazole**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20810-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Bifonazole; Bifonazolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Bifonazole*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Bifonazole	1206027-01	20810	40	1312397
Fagron	Bifonazole	12G11-N09	20820	40	20120807
Euro OTC	Bifonazole	1401031-01	21631	40	20140220
Euro OTC	Bifonazole	1510001	22253	40	20151203*
Caelo	Bifonazole	15152701	22906	40	20150703
Caelo	Bifonazole	15152702	22907	40	20150703
Fagron	Bifonazole	16D07-B10-324381	22941	40	20160419

Validation samples

A total of 280 317 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 *Bifonazole*. These samples are listed above in the [calibration samples](#) section.
- 74 216 spectra from a total of 1616 batches from further 372 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 8 reference samples from the substance/substance group *Bifonazole*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Bifonazole	1401031-01	21631 [†]	20
Euro OTC	Bifonazole	1510001	22253 [†]	20
Caelo	Bifonazole	15152702	22955	40
Caelo	Bifonazole	151527	23364	40
Euro OTC	Bifonazole	1703041	23395	40
Euro OTC	Bifonazole	1806008	24161	40
Caelo	Bifonazole	182771	24365	40
Euro OTC	Bifonazole	1510001	22253SI	60

- 126 592 spectra from a total of 2782 batches from further 781 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.

- 46 spectra from 27 *Apo-Ident* customers from 25 batches from the substance/substance group *Bifonazole*.

Supplier	Substance	Batch	Spectra
Fagron	Bifonazole	11F20-N06	1
Fagron	Bifonazole	12E29-N03	5
Euro OTC	Bifonazole	1206027-01	2
Fagron	Bifonazole	12G11-N09	2
Euro OTC	Bifonazole	1206027-02	1
Euro OTC	Bifonazole	13G10N02	1
Fagron	Bifonazole	13G10-N02	2
Fagron	Bifonazole	14C28-B03-292388	1
Fargon	Bifonazole	14k10-b01-300541	1
Fagron	Bifonazole	14K10-B01-300541	6
Fagron	Bifonazole	14K10-B01-306783	4
Fagron	Bifonazole	14K10-B01-308349	2
Fagron	Bifonazole	14K10-B01-312067	2
Caelo	Bifonazole	15152701	1
Euro OTC	Bifonazole	1510001-02	4
Fagron	Bifonazole	14K10-B01-316618	1
Fagron	Bifonazole	16D07-B10-32480	1
Fagron	Bifonazole	16D07-B10-324380	1
Fagron	Bifonazole	16D07-B10-321576	1
Caelo	Bifonazole	14k10-B01-312067	1
Gehe	Bifonazole	15152703	1
Fagron	Bifonazole	16J03-B08-327046	1
Caelo	Bifonazole	18009702	2
Fagron	Bifonazole	16J03-B08-333936	1
Euro OTC	Bifonazole	1703041-01	1

- 78 883 spectra from 565 *Apo-Ident* customers from a total of 26 112 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Bifonazole* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bifonazole* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 216
Type B	0	300	0	126 592
Type C	0	46	0	78 883

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 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
20810	20810	0.00	38.83
21631	22253	4.55	39.59
22253	22253	0.00	44.65
22906	20810	4.24	38.38
22907	20810	4.59	37.46
22941	20810	3.77	37.05
20820	20810	8.42	35.37

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Biotin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20414-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Biotin; Biotinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Biotin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Biotin	13K29-N02	21221	40	20131204
Euro OTC	Biotin	1402028-01	21632	40	20140404
Euro OTC	Biotin	1508030	21904	40	20150925*
Euro OTC	Biotin	1610003	22855	40	20161110*
Caelo	Biotin	16164313	22902	40	20160216

Validation samples

A total of 280 317 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 *Biotin*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1618 batches from further 372 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 10 reference samples from the substance/substance group *Biotin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Biotin	1402028-01	21632 [†]	20
Euro OTC	Biotin	1508030	21904 [†]	20
Euro OTC	Biotin	1603017	22507	40
Caelo	Biotin	16164313	22901	40
Caelo	Biotin	163432	23029	40
Caelo	Biotin	163432	23063	40
Euro OTC	Biotin	1708007	23728	40
Caelo	Biotin	173152	23829	40
Euro OTC	Biotin	1802022	23955	40
Caelo	Biotin	183009	24372	40

- 126 532 spectra from a total of 2780 batches from further 781 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.

- 34 spectra from 15 *Apo-Ident* customers from 23 batches from the substance/substance group *Biotin*.

Supplier	Substance	Batch	Spectra
Fagron	Biotin	13081203	1
Fagron	Biotin	13111202	1
Euro OTC	Biotin	1111039-02	1
Euro OTC	Biotin	1301026-01	3
Caelo	Biotin	12A23-N03	1
Fagron	Biotin	13K29-N02	2
Fagron	Biotin	12111302	1
Fagron	Biotin	20110634	1
Fagron	Biotin	14d04-b07-292963	1
Fagron	Biotin	12C14-N01	1
Fagron	Biotin	12A23-N03	1
Euro OTC	Biotin	2041517	1
Euro OTC	Biotin	1402028-01	2
Euro OTC	Biotin	3021501	1
Euro OTC	Biotin	28071506	1
Euro OTC	Biotin	1411047-01	1
Caelo	Biotin	1402028-01	2
Euro OTC	Biotin	1610003-01	3
Euro OTC	Biotin	10061709	1
Euro OTC	Biotin	1708007-01	1
Euro OTC	Biotin	24011801	1
Euro OTC	Biotin	161000301	1
Euro OTC	Biotin	1802022-01	2
Fagron	Biotin	17K20-B03-351524	1
EuRho	Biotin	1802022-01	1
Euro OTC	Biotin	5121812	1

- 78 895 spectra from 565 *Apo-Ident* customers from a total of 26 114 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Biotin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Biotin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	360	0	126 532
Type C	0	34	0	78 895

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 82.3529 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21221	21904	9.73	76.17
21632	21904	5.07	70.34
21904	21904	0.00	73.37
22855	22855	0.00	72.74
22902	21904	4.14	68.53

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Bismuth gallath, basic**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21252-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Bismuth gallath, basic; Bismuthi subgallas

Special notes

When selecting the *Bismuth gallath, basic* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Bismuth gallath, basic*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Bismuth gallath,...	13179105	21252	40	1412254
Fagron	Bismuth gallath,...	15B02-B04-309481	22597	40	20150226
Caelo	Bismuth gallath,...	17004102	23372	40	20170214
Fagron	Bismuth gallath,...	16K17-B04-335597	23570	40	20170623

Validation samples

A total of 280317 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 *Bismuth gallath, basic*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 3 reference samples from the substance/substance group *Bismuth gallath, basic*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Bismuth gallath, basic	13179105	21553	60
Fagron	Bismuth gallath, basic	15J26-B02-317883	22598	40
Caelo	Bismuth gallath, basic	170041	23359	40

- 126752 spectra from a total of 2786 batches from further 781 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.

- 333 spectra from 171 *Apo-Ident* customers from 137 batches from the substance/substance group *Bismuth gallath, basic*.

Supplier	Substance	Batch	Spectra
Caelo	Bismuth gallath, basic	92057409	1
Fagron	Bismuth gallath, basic	10H31-N01	1

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Supplier	Substance	Batch	Spectra
Caelo	Bismuth gallath, basic	12166901	2
Fagron	Bismuth gallath, basic	2010002685	2
Anzag	Bismuth gallath, basic	2012000059	2
Caelo	Bismuth gallath, basic	81297468	5
Fagron	Bismuth gallath, basic	2012000059	3
Phoenix, Jembke	Bismuth gallath, basic	10135101	1
Caelo	Bismuth gallath, basic	12I13-N11	1
Klenk	Bismuth gallath, basic	12E16-N03	1
Fagron	Bismuth gallath, basic	11F15-N03	1
Caelo	Bismuth gallath, basic	12C13-N03	1
Caelo	Bismuth gallath, basic	1127203	1
Caelo	Bismuth gallath, basic	12E16-N03	1
Caelo	Bismuth gallath, basic	8129768	1
Fagron	Bismuth gallath, basic	12C13-N03	4
Phönix	Bismuth gallath, basic	12-13-N11	1
Fagron	Bismuth gallath, basic	12K26-N01	3
Caelo	Bismuth gallath, basic	9205703	2
Caelo	Bismuth gallath, basic	5208I-01185	1
Fagron	Bismuth gallath, basic	12/13-N11	1
Phönix	Bismuth gallath, basic	12E16-N03	1
Caelo	Bismuth gallath, basic	12172401	1
Caelo	Bismuth gallath, basic	B-150513-1	1
Fagron	Bismuth gallath, basic	13D19-N02	3
Caelo	Bismuth gallath, basic	12172409	6
Caelo	Bismuth gallath, basic	12c13-n03	1
Caelo	Bismuth gallath, basic	12172402	4
Sanacorp	Bismuth gallath, basic	12/13-N11	1
Sanacorp	Bismuth gallath, basic	13D19-N02	1
Alliance	Bismuth gallath, basic	12172402	1
Apomix/Noweda	Bismuth gallath, basic	13D19-N02	1
Caelo	Bismuth gallath, basic	13D19-N02	2
Caelo	Bismuth gallath, basic	1217240	1
Gehe	Bismuth gallath, basic	12172401	1
Caelo	Bismuth gallath, basic	10D23-N05	1
Alliance Healthcare	Bismuth gallath, basic	13D19-N02	2
Fagron	Bismuth gallath, basic	12E16-N03	1
Caelo	Bismuth gallath, basic	9205701	1
Fagron	Bismuth gallath, basic	2012006724	2
Fagron	Bismuth gallath, basic	13E21-N03	1
PHOENIX am 17.01.2014	Bismuth gallath, basic	2012006724	1
Fagron	Bismuth gallath, basic	411092-3-P	1
siehe WE-Prüfprotokoll	Bismuth gallath, basic	4/09	1
Fargron	Bismuth gallath, basic	13D19-N02	1
Fagron	Bismuth gallath, basic	13G10-N12	4
Caelo	Bismuth gallath, basic	12c13-no3	1
Fagron	Bismuth gallath, basic	13K08-N03	3
ahd/lamotte	Bismuth gallath, basic	13718b13292058	1
Caelo	Bismuth gallath, basic	13179101	1
Fagron	Bismuth gallath, basic	13/18-B13-292058	1
Caelo	Bismuth gallath, basic	13/18-B13-292057	1
Caelo	Bismuth gallath, basic	13179111	6
Caelo	Bismuth gallath, basic	2414E-01185	1
Fagron	Bismuth gallath, basic	13/18-B13-292057	2
Bombastus	Bismuth gallath, basic	13/18-B13-292058	1
Fagron	Bismuth gallath, basic	1318-B13-292057	2
Fagron	Bismuth gallath, basic	13I18-B13-292057	1
Bombastus	Bismuth gallath, basic	13G10-N12	1
Fagron	Bismuth gallath, basic	13I18-B13-292058	1
Fagron	Bismuth gallath, basic	5121	1
Fagron	Bismuth gallath, basic	1318b13292058	1

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Supplier	Substance	Batch	Spectra
Fagron	Bismuth gallath, basic	13I18-B13	5
Caelo	Bismuth gallath, basic	13/18-B13-292058	1
Fagron	Bismuth gallath, basic	13179111	1
sanacorp	Bismuth gallath, basic	13/1818B13-292057	1
Fagron	Bismuth gallath, basic		1
Fagron	Bismuth gallath, basic	13I18-B13-294098	4
Caelo	Bismuth gallath, basic	23121410	1
Fagron	Bismuth gallath, basic	13/18-B13-294108	3
Fagron	Bismuth gallath, basic	13/18-B-13-292057	1
Caelo	Bismuth gallath, basic	13179105	1
Fagron	Bismuth gallath, basic	13/18-B13-294098	1
Caelo	Bismuth gallath, basic	14224103	4
Caelo	Bismuth gallath, basic	2012006724	1
Fagron	Bismuth gallath, basic	13/18-B13294098	1
Infectopharm	Bismuth gallath, basic	14224103	1
Fagron	Bismuth gallath, basic	13I18-b13-292057	1
Fagron	Bismuth gallath, basic	1318B13294108	1
Fagron	Bismuth gallath, basic	13i18-b13-294108	1
Caelo	Bismuth gallath, basic	11127104	1
Fagron	Bismuth gallath, basic	13I18-B13-294108	5
Martinus Apotheke	Bismuth gallath, basic	keine	1
Fagron	Bismuth gallath, basic	13/18-B13-294108	1
Fagron	Bismuth gallath, basic	15B02-B04-304408	7
Fagron	Bismuth gallath, basic	14H13-B07-303639	6
Fagron	Bismuth gallath, basic	14H13B07303639	1
Caelo	Bismuth gallath, basic	13I18-B13-294108	1
Caelo	Bismuth gallath, basic	15080602	3
Caelo	Bismuth gallath, basic	12172412	3
Caelo	Bismuth gallath, basic	13I18-B13	1
Fagron	Bismuth gallath, basic	12B02-B04-304408	1
Fagron	Bismuth gallath, basic	15b02b04304408	1
Caelo	Bismuth gallath, basic	15B02B04304413	1
Fagron	Bismuth gallath, basic	15B02-B04-304413	5
Fagron	Bismuth gallath, basic	14H13-B07	1
Caelo	Bismuth gallath, basic	15080606	7
Fagron	Bismuth gallath, basic	2014006082	1
Caelo	Bismuth gallath, basic	1520910	1
Caelo	Bismuth gallath, basic	15200907	1
Fagron	Bismuth gallath, basic	15B02-B04-311878	1
Fagron	Bismuth gallath, basic	15B02-B04	2
Caelo	Bismuth gallath, basic	15B02-B04-309481	2
Caelo	Bismuth gallath, basic	15080603	1
Caelo	Bismuth gallath, basic	10135109	1
Fagron	Bismuth gallath, basic	15b02-B04-309481	1
Alliance H.	Bismuth gallath, basic	15080602	1
Caelo	Bismuth gallath, basic	15200913	3
Fagron	Bismuth gallath, basic	15C27-B02-311879	1
Fargon/ Noweda	Bismuth gallath, basic	15B02-B04-309481	1
Fagron	Bismuth gallath, basic	15B02-B04-309481	1
Fagron	Bismuth gallath, basic	2015000866	1
Caelo	Bismuth gallath, basic		1
Caelo	Bismuth gallath, basic	15200904	2
Fagron	Bismuth gallath, basic	15H05-B07	1
Caelo	Bismuth gallath, basic	1520913	1
Fagron	Bismuth gallath, basic	15J26-B02-320473	5
Fagron	Bismuth gallath, basic	15J26-B02-317883	6
Caelo	Bismuth gallath, basic	15200905	1
Phoenix	Bismuth gallath, basic	1520913	1
Caelo	Bismuth gallath, basic	16038308	5
Fagron	Bismuth gallath, basic	15J26-B02-321313	5

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Supplier	Substance	Batch	Spectra
Fagron	Bismuth gallath, basic	15H05-B07-311880	4
Fagron	Bismuth gallath, basic	15B02-B04-209481	1
Fagron	Bismuth gallath, basic	2015007568	4
Caelo	Bismuth gallath, basic	9K26-N10	2
Fargon GmbH & Co.KG	Bismuth gallath, basic	15J26-B02-321313	2
Fagron	Bismuth gallath, basic	15J26-B02	2
Caelo	Bismuth gallath, basic	15200911	4
Fagron	Bismuth gallath, basic	15/26-B02-320473	1
Caelo	Bismuth gallath, basic	15J26B02-321313	1
Fagron	Bismuth gallath, basic	325472	1
Caelo	Bismuth gallath, basic	16038310	4
Fagron	Bismuth gallath, basic	15J26-B02-325472	4
phönix	Bismuth gallath, basic	15J26-B02-325450	1
Caelo	Bismuth gallath, basic	17004102	6
Allianz Healthcare	Bismuth gallath, basic	15200911	1
Caelo	Bismuth gallath, basic	15J26-B02-320473	1
Caelo	Bismuth gallath, basic	16038312	6
Fagron	Bismuth gallath, basic	15J26-B02-325450	1
Fagron	Bismuth gallath, basic	2015000361	1
Fagron	Bismuth gallath, basic	15J26-B022	1
Caesar & Loretz GmbH	Bismuth gallath, basic	17004102	1
Fagron	Bismuth gallath, basic	16K17-B04-335597	6
Caelo	Bismuth gallath, basic	16K17-B04-335597	1
Caelo	Bismuth gallath, basic	17004106	7
Sidonia	Bismuth gallath, basic	15J-26-B02-325450	1
Sidonia	Bismuth gallath, basic	15200904	1
Fagron	Bismuth gallath, basic	16K17-B04	1
Frago/Noweda	Bismuth gallath, basic	16K17-B04-335597	1
Sidonia	Bismuth gallath, basic	17004107	2
Caelo	Bismuth gallath, basic	2017002570	1
Caelo	Bismuth gallath, basic	17004109	3
Caelo	Bismuth gallath, basic	17004107	3
Fragon/Sanacorp	Bismuth gallath, basic	16K17-B04-335593	1
Fagron	Bismuth gallath, basic	17E16-B02	1
Fagron	Bismuth gallath, basic	17/26-B01-340556	3
Caelo	Bismuth gallath, basic	17004112	5
Fagron	Bismuth gallath, basic	2016006984	1
Fagron	Bismuth gallath, basic	17I26-B01-340556	3
Fagron	Bismuth gallath, basic	180307BB/2016006984	1
Fagron	Bismuth gallath, basic	2017006945	2
Fragon/Sanacorp	Bismuth gallath, basic	17/26-B01-340552	1
Fagron	Bismuth gallath, basic	17I26-B01-341866	3
Fagron	Bismuth gallath, basic	18A29-B06-346303	1
Fragon/Sanacorp	Bismuth gallath, basic	18A-29-B06-346303	1
Fagron	Bismuth gallath, basic	18A29-B06-3460303	1
Caelo	Bismuth gallath, basic	17259503	1
Caelo	Bismuth gallath, basic	18A29-B06	1
Caelo	Bismuth gallath, basic	18A29-B06-346305	1
Caelo	Bismuth gallath, basic	17259509	2
Caelo	Bismuth gallath, basic	18040801	1
Caelo	Bismuth gallath, basic	1725909	1
Kehr	Bismuth gallath, basic	17I26-B01-341866	1

- 78 596 spectra from 565 *Apo-Ident* customers from a total of 26 001 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#),

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

Validation results

The validation runs checked whether the substance/substance group *Bismuth gallath, basic* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bismuth gallath, basic* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	120	20	126 752
Type C	0	311	22	78 596

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	85.7143 % (> 83.5714 %)
Type C	100.0000 % (> 99.8817 %)	93.3934 % (> 92.4925 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21252	21252	0.00	107.17
22597	21252	3.17	110.35
23372	21252	2.43	118.75
23570	21252	3.91	112.72

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Boric acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20182-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Boric acid; Acidum boricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Boric acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Boric acid	13I04-N06	21228	40	20130920
Caelo	Boric acid	14133119	21804	40	20140509
Caelo	Boric acid	15425112	22964	40	20160104
Caelo	Boric acid	170613	23286	40	20170316*

Validation samples

A total of 280317 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 *Boric acid*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 *Boric acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Boric acid	14133119	21804 [†]	20
Caelo	Boric acid	15242903	22965	40
Fagron	Boric acid	15L09-B07-322988	23746	40

- 126792 spectra from a total of 2786 batches from further 781 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 24 *Apo-Ident* customers from 31 batches from the substance/substance group *Boric acid*.

*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	Boric acid	9324036	1
Fagron	Boric acid	11I26-n05	1
Fagron	Boric acid	12f01-n08	1
Caelo	Boric acid	11D13-N08	1
Fagron	Boric acid	11d13-n08	1
Caelo	Boric acid	9324043	1
Caelo	Boric acid	12260502	1
Caelo	Boric acid	12238901	1
Nachprüfung	Boric acid		1
Fagron	Boric acid	12G04-N10	1
Caelo	Boric acid	10227913	1
Fagron	Boric acid	14133101	1
Fagron	Boric acid	13I04-N06	2
Caelo	Boric acid	14095202	1
Sanacorp	Boric acid	1/AKD3	1
Caelo	Boric acid	14133113	2
Fagron	Boric acid	14B07-B02-295752	1
Caelo	Boric acid	9324021	1
Caelo	Boric acid	15095103	2
Caelo	Boric acid	14133119	1
Caelo	Boric acid	15158903	1
Caelo	Boric acid	15158901	1
Caelo	Boric acid	15425101	4
Caelo	Boric acid	15425108	2
Caelo	Boric acid	80303AB	1
Caelo	Boric acid	15425114	1
Caelo	Boric acid	15425118	2
Caelo	Boric acid	15242906	1
Caelo	Boric acid	5425114	1
Caelo	Boric acid	15425112	1
Caelo	Boric acid	15242909	1

- 78 890 spectra from 565 *Apo-Ident* customers from a total of 26 107 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Boric 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 *Boric 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	160	0	74 336
Type B	0	100	0	126 792
Type C	0	39	0	78 890

The substance/substance group *Boric 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 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 84.6154 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21228	23286	13.51	54.96
21804	23286	17.12	55.29
22964	23286	8.63	54.85
23286	23286	0.00	54.49

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Budesonide, micronized**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20569-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Budesonide, micronized; Budesonidum micronisatum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Budesonide, micronized*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Budesonide, micr...	11351704	20808	40	AR-15-FG-005286-01
Euro OTC	Budesonide, micr...	1311022-01	21620	40	20140113
Euro OTC	Budesonide, micr...	1604018	22537	40	20160509*
Caelo	Budesonide, micr...	161431	22627	40	20160606*
Caelo	Budesonide, micr...	15344004	22649	40	20151116

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Budesonide, micr...	16J04-B01-326581	22888	40	20161026
Euro OTC	Budesonide, micr...	1311022-01	21620SI	25	20140113
Euro OTC	Budesonide, micr...	1604018	22537SI	23	20160509*
Caelo	Budesonide, micr...	161431	22627SI	25	20160606*
Caelo	Budesonide, micr...	15344004	22649SI	23	20151116
Fagron	Budesonide, micr...	16J04-B01-326581	22888SI	30	20161026

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 366 spectra of 11 reference samples from the substance/substance group *Budesonide, micronized*. These samples are listed above in the [calibration samples](#) section.
- 74 130 spectra from a total of 1617 batches from further 372 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 [†].

- 323 spectra of 12 reference samples from the substance/substance group *Budesonide, micronized*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Budesonide, micronized	11351706	20800	40
Euro OTC	Budesonide, micronized	1311022-01	21620 [†]	20
Fagron	Budesonide, micronized	16J04-B01-326581	22841	40
Caelo	Budesonide, micronized	170788	23279	40
Euro OTC	Budesonide, micronized	1709022	23778	40
Caelo	Budesonide, micronized	180749	24026	40
Euro OTC	Budesonide, micronized	1311022-01	21620SI [†]	12
Caelo	Budesonide, micronized	15344004	22649SI [†]	7
Fagron	Budesonide, micronized	16J04-B01-326581	22841SI	24
Caelo	Budesonide, micronized	170788	23279SI	20
Euro OTC	Budesonide, micronized	1709022	23778SI	20
Caelo	Budesonide, micronized	180749	24026SI	20

*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.

- 126 569 spectra from a total of 2782 batches from further 781 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.

- 149 spectra from 61 *Apo-Ident* customers from 75 batches from the substance/substance group *Budesonide, micronized*.

Supplier	Substance	Batch	Spectra
Caelo	Budesonide, micronized	11175014	2
Caelo	Budesonide, micronized	11351707	3
Fagron	Budesonide, micronized	12G23-N01	2
Caelo	Budesonide, micronized	11351706	4
Caelo	Budesonide, micronized	11351701	1
Caelo	Budesonide, micronized	21100M1	1
Caelo	Budesonide, micronized	11351703	1
Caelo	Budesonide, micronized	12295103	1
Fagron	Budesonide, micronized	13A07-N09	1
Caelo	Budesonide, micronized	11351713	1
Caelo	Budesonide, micronized	12295109	2
Caelo	Budesonide, micronized	11175015	1
Caelo	Budesonide, micronized	12295105	1
crystal pharma/gehe	Budesonide, micronized	1305004-01	2
Caelo	Budesonide, micronized	12295106	2
Fagron	Budesonide, micronized	14A30-B09-291366	2
Fagron	Budesonide, micronized	13H22-N03	1
Caelo	Budesonide, micronized	12295108	1
Phoenix	Budesonide, micronized	14071702	3
Caelo	Budesonide, micronized	14071701	1
Caelo	Budesonide, micronized	14071702	5
Caelo	Budesonide, micronized	12295111	2
VDI 23.10.14 19,50 euro	Budesonide, micronized	14071707	1
Caelo	Budesonide, micronized	12295110	4
Fagron	Budesonide, micronized	14A30-B09291366	1
Fagron	Budesonide, micronized	14H15-B02	3
Caelo	Budesonide, micronized	14071707	2
sanacorp	Budesonide, micronized	14071701	1
Caelo	Budesonide, micronized	14071717	3
Caelo	Budesonide, micronized	14071714	4
Fagron	Budesonide, micronized	14H15-B02-297926	1
Euro OTC	Budesonide, micronized	1311022-01	3
Caelo	Budesonide, micronized	1471707	1
Fagron	Budesonide, micronized	14H15-B02-301971	2
Caelo	Budesonide, micronized	15173806	2
Caelo	Budesonide, micronized	15173803	3
Fagron	Budesonide, micronized	15E27-B01-308321	1
Fagron	Budesonide, micronized	14H15-B02-301972	1
Caelo	Budesonide, micronized	15344003	6

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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	Budesonide, micronized	15E27-B10-308322	1
Caelo	Budesonide, micronized	15173810	1
Caelo	Budesonide, micronized	15173811	4
Caelo	Budesonide, micronized	15173807	3
Fagron	Budesonide, micronized	15E27B10	1
Caelo	Budesonide, micronized	15173802	2
Fagron	Budesonide, micronized	15E27-B10-315704	1
Caelo	Budesonide, micronized	15344002	1
Caelo	Budesonide, micronized	15044002	1
Caelo	Budesonide, micronized	15344006	1
Caelo	Budesonide, micronized	15344010	3
Caelo	Budesonide, micronized	15344012	2
Caelo	Budesonide, micronized	15344008	5
Fagron	Budesonide, micronized	15344012	1
Caelo	Budesonide, micronized	15344013	1
Caelo	Budesonide, micronized	15344014	1
Caelo	Budesonide, micronized	16143102	1
Caelo	Budesonide, micronized	15344005	2
Sanacorp,	Budesonide, micronized	16143103	1
Caelo	Budesonide, micronized	16143108	2
Caelo	Budesonide, micronized	16143101	1
Caelo	Budesonide, micronized	16143107	2
Noweda	Budesonide, micronized	16143108	1
Fagron	Budesonide, micronized	17A17-B01-331248	1
Fargon/Kehr	Budesonide, micronized	16J04-B01-326583	1
Caelo	Budesonide, micronized	170078801	1
Noweda	Budesonide, micronized	16143110	1
Caelo	Budesonide, micronized	16143112	2
Caelo	Budesonide, micronized	17078804	1
Caelo	Budesonide, micronized	17078801	6
Caelo	Budesonide, micronized	17078804	1
Caelo	Budesonide, micronized	17078809	1
Caelo	Budesonide, micronized	17078803	2
Caelo	Budesonide, micronized	17078808	4
Euro OTC	Budesonide, micronized	1604018-01	1
Caelo	Budesonide, micronized	18074901	1
Fagron	Budesonide, micronized	17A17-B01-331448	1
Caelo	Budesonide, micronized	18074903	1
Caelo	Budesonide, micronized	17078805	2
Caelo	Budesonide, micronized	17342902	1
Fagron	Budesonide, micronized	18074901	1
Caelo	Budesonide, micronized	18074905	1
Fagron	Budesonide, micronized	18172601	1

- 78 780 spectra from 565 *Apo-Ident* customers from a total of 26 063 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

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

	False positive	True positive	False negative	True negative
Type A	0	366	0	74 130
Type B	0	323	0	126 569
Type C	0	149	0	78 780

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.3607 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.1424 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 95.9732 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22537	22537	0.00	30.46
21620	20808	4.34	35.16
22627	22627	0.00	31.55
20808	20808	0.00	40.86
22649	22627	3.64	32.67
22888	22627	2.94	32.82

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Butylated hydroxytoluene**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21307-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Butylated hydroxytoluene; Butylhydroxytoluenum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Butylated hydroxytoluene*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Butylated hydrox...	13354602	21307	40	20131105
Caelo	Butylated hydrox...	13354604	21355	40	AR-15-FG-007846-02
Caelo	Butylated hydrox...	15172103	22350	40	20150529

Validation samples

A total of 280 317 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 *Butylated hydroxytoluene*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Butylated hydroxytoluene*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Butylated hydroxytoluene	15172103	21911	60
Caelo	Butylated hydroxytoluene	15172103	22281	60
Caelo	Butylated hydroxytoluene	15172103	22350 [†]	20
Caelo	Butylated hydroxytoluene	163163	23356	40
Caelo	Butylated hydroxytoluene	180291	24019	40

- 126 672 spectra from a total of 2786 batches from further 781 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.

- 229 spectra from 169 *Apo-Ident* customers from 51 batches from the substance/substance group *Butylated hydroxytoluene*.

[†]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	Butylated hydroxytoluene	11131006	1
Fagron	Butylated hydroxytoluene	11308701	1
Noweda	Butylated hydroxytoluene	12158201	1
Caelo	Butylated hydroxytoluene	12158201	3
Caelo	Butylated hydroxytoluene	12158204	5
Caelo	Butylated hydroxytoluene	20161112-1	1
Caelo	Butylated hydroxytoluene	1220705	1
Caelo	Butylated hydroxytoluene	12280203	5
Caelo	Butylated hydroxytoluene	122080206	1
Caelo	Butylated hydroxytoluene	12280201	1
Caelo	Butylated hydroxytoluene	12207005	3
Caelo	Butylated hydroxytoluene	12280206	4
Caelo	Butylated hydroxytoluene	12382302	5
Caelo	Butylated hydroxytoluene	2113U02851	1
Caelo	Butylated hydroxytoluene	12382304	7
Noweda	Butylated hydroxytoluene	12382304	1
Caelo	Butylated hydroxytoluene	12382307	1
Caelo	Butylated hydroxytoluene	12382309	7
Caelo	Butylated hydroxytoluene	7031403	1
Phoenix	Butylated hydroxytoluene	3111201	1
Phoenix	Butylated hydroxytoluene	12382305	1
Caelo	Butylated hydroxytoluene	13354602	4
Caelo	Butylated hydroxytoluene	12382312	1
Caelo	Butylated hydroxytoluene	13354604	8
Bombastus	Butylated hydroxytoluene	13354604	1
Phoenix	Butylated hydroxytoluene	13354609	1
Caelo	Butylated hydroxytoluene	13354611	3
Caelo	Butylated hydroxytoluene	14300501	10
Caelo	Butylated hydroxytoluene	1400501	1
Caelo	Butylated hydroxytoluene	14300502	5
Caelo	Butylated hydroxytoluene	143004502	1
Caelo	Butylated hydroxytoluene	14300506	1
Caelo	Butylated hydroxytoluene	13354609	2
Caelo	Butylated hydroxytoluene	14300505	6
Caelo	Butylated hydroxytoluene	15094501	8
Sanacorp	Butylated hydroxytoluene	14300505	1
Caelo	Butylated hydroxytoluene	15172101	9
Caelo	Butylated hydroxytoluene	15172103	18
sanacorp	Butylated hydroxytoluene	15172103	1
Noweda	Butylated hydroxytoluene	15172103	1
Caelo	Butylated hydroxytoluene	15172105	10
Fagron	Butylated hydroxytoluene	15426801	1
Phoenix	Butylated hydroxytoluene	15426801	1
Caelo	Butylated hydroxytoluene	15426801	7
Caelo	Butylated hydroxytoluene	231115BHT	1
Celo	Butylated hydroxytoluene	15426801	1
Caesar & Loretz	Butylated hydroxytoluene	15426801	1
Caelo	Butylated hydroxytoluene	1426801	1
Caelo	Butylated hydroxytoluene	716M-02851	1
Caelo	Butylated hydroxytoluene	16316301	8
Caelo	Butylated hydroxytoluene	15426807	10
Gehe	Butylated hydroxytoluene	15426807	1
Caelo	Butylated hydroxytoluene	2170717	1
Caelo	Butylated hydroxytoluene	1631301	1
Caelo	Butylated hydroxytoluene	16316305	8
Caelo	Butylated hydroxytoluene	163163055402	1
Caelo	Butylated hydroxytoluene	16316304	7
Noweda	Butylated hydroxytoluene	16316305	1
Sanacorp	Butylated hydroxytoluene	16316305	1
SanacorpWE:04.01.18 E....	Butylated hydroxytoluene	16316304	1

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Supplier	Substance	Batch	Spectra
Caelo	Butylated hydroxytoluene	16316307	10
Caelo	Butylated hydroxytoluene	18048701	6
Caelo	Butylated hydroxytoluene	18029102	7
AHD	Butylated hydroxytoluene	18029102	1
Caelo	Butylated hydroxytoluene	16316304-20180619Ma5	1
Apo Ident/ Noweda	Butylated hydroxytoluene	18029104	1
Caelo	Butylated hydroxytoluene	18029105	5

- 78 700 spectra from 565 *Apo-Ident* customers from a total of 26 087 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Butylated hydroxytoluene* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Butylated hydroxytoluene* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	220	0	126 672
Type C	0	220	9	78 700

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.8817 %)	96.0699 % (> 94.7598 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21307	21355	3.02	68.09
21355	21355	0.00	67.68
22350	21355	1.83	66.13

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Caffeine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20962-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Caffeine; Coffeinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Caffeine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Caffeine	1211012-01	20962	40	1412248
Caelo	Caffeine	12317911	21205	40	20121113
Caelo	Caffeine	13233105	21456	40	20131008
Caelo	Caffeine	13233104	21548	40	20131008

Validation samples

A total of 280 317 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 *Caffeine*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 7 reference samples from the substance/substance group *Caffeine*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Caffeine	12317911	21089	40
Caelo	Caffeine	13233105	21456 [†]	20
Caelo	Caffeine	13233104	21548 [†]	20
Euro OTC	Caffeine	1603009	22517	40
Caelo	Caffeine	15082303	22823	40
Euro OTC	Caffeine	1703006	23140	40
Euro OTC	Caffeine	1808017	24199	40

- 126 652 spectra from a total of 2782 batches from further 781 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.

- 112 spectra from 70 *Apo-Ident* customers from 49 batches from the substance/substance group *Caffeine*.

[†]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	Caffeine	11076807	2
Caelo	Caffeine	12093410	2
Caelo	Caffeine	12317904	2
EUro/AHD	Caffeine	121012-01	1
Caelo	Caffeine	12317902	1
Caelo	Caffeine	9301807	1
Caelo	Caffeine	12093418	2
Euro OTC	Caffeine	1211012-01	1
Euro OTC	Caffeine	1211012-02	1
Caelo	Caffeine	12317906	1
Caelo	Caffeine	12317909	7
Euro OTC	Caffeine	1307049-01	5
EUro/AHD	Caffeine	1307049-01	1
Caelo	Caffeine	12317914	2
Gatt-Koller / Phoenix	Caffeine	5898/12135213	2
Euro OTC	Caffeine	26081406	1
Noweda	Caffeine	1404026-01	1
Caelo	Caffeine	13233105	4
Caelo	Caffeine	3212E-01281	1
Caelo	Caffeine	12093402	2
Euro OTC	Caffeine	1109017-01	1
Caelo	Caffeine	13233111	5
Euro OTC	Caffeine	1411015-01	4
Euro OTC	Caffeine	325241AX20	1
Caelo	Caffeine	1211012-01	1
Caelo	Caffeine	15054704	2
ACM	Caffeine	KNC1294J14	2
Caelo	Caffeine	1503020-01	2
Euro OTC	Caffeine	1503020-01	5
Caelo	Caffeine	15054709	1
Fagron	Caffeine	15H11-B02	1
Euro OTC	Caffeine	1503020-02	7
Euro OTC	Caffeine	160300901	2
Caelo	Caffeine	15082311	1
Euro OTC	Caffeine	1603009-01	2
Caelo	Caffeine	15375006	2
Euro OTC	Caffeine	1603009-02	3
Caelo	Caffeine	11111111	1
Phönix	Caffeine	1603009-02	1
Euro/Noweda	Caffeine	1703006-01	1
Euro OTC	Caffeine	1703006-01	10
Euro OTC	Caffeine	1603009/01	1
Caelo	Caffeine	15375007	1
Caelo	Caffeine	15375012	2
Caelo	Caffeine	15082315	1
Caelo	Caffeine	15372012	1
Euro OTC	Caffeine	16462119	1
Merck	Caffeine	MerckReagenziensatz	1
Caelo	Caffeine	17173707	1
Caelo	Caffeine	18011901	3
Euro OTC	Caffeine	1703006-02	2
Caelo	Caffeine	18011902	1
Caelo	Caffeine	18077906	1
Caelo	Caffeine	18011906	1

- 78 817 spectra from 565 *Apo-Ident* customers from a total of 26 088 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#),

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

Validation results

The validation runs checked whether the substance/substance group *Caffeine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Caffeine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	240	0	126 652
Type C	0	109	3	78 817

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.8817 %)	97.3214 % (> 94.6429 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20962	20962	0.00	95.52
21205	20962	2.47	95.84
21456	20962	5.28	95.31
21548	20962	2.96	95.01

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Calcium ascorbate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20393-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Calcium ascorbate; Calcii ascorbinicum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Calcium ascorbate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium ascorbate	13105624	21313	40	20130620
Euro OTC	Calcium ascorbate	1612003	22916	40	20170110*
Euro OTC	Calcium ascorbate	1709005	23609	40	20170914*
Euro OTC	Calcium ascorbate	1709004	23611	40	20170914*
Euro OTC	Calcium ascorbate	1801010	23884	40	20180115*

Validation samples

A total of 280 317 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 *Calcium ascorbate*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1618 batches from further 372 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 *Calcium ascorbate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Calcium ascorbate	1607033-01	22812	40
Caelo	Calcium ascorbate	163111	23060	40
Caelo	Calcium ascorbate	16311101	23518	40
Euro OTC	Calcium ascorbate	1807032	24194	40
Caelo	Calcium ascorbate	183226	24373	40

- 126 692 spectra from a total of 2784 batches from further 781 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.

- 10 spectra from 6 *Apo-Ident* customers from 10 batches from the substance/substance group *Calcium ascorbate*.

*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
Farmalabor / Farmalabor	Calcium ascorbate	P1104931-000A	1
Caelo	Calcium ascorbate	13105608	1
Caelo	Calcium ascorbate	14340907	1
Burton Feingold	Calcium ascorbate	L008415	1
Caelo	Calcium ascorbate	15324708	1
Arktis	Calcium ascorbate	7339/4617	1
Euro OTC	Calcium ascorbate	1801010	1
Euro OTC	Calcium ascorbate	1709005	1
Arktis	Calcium ascorbate	733P/1518	1
Euro OTC	Calcium ascorbate	1709004-01	1

- 78 919 spectra from 565 *Apo-Ident* customers from a total of 26 127 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Calcium ascorbate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium ascorbate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	200	0	126 692
Type C	0	10	0	78 919

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8818 %)	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
23611	23611	0.00	31.76
23884	23884	0.00	33.34
21313	22916	6.42	30.80
22916	22916	0.00	31.86
23609	23609	0.00	31.78

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Calcium citrate tetrahydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20013-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium citrate tetrahydrate; Calcii citras tetrahydricus

Special notes

When selecting the *Calcium citrate tetrahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Calcium citrate tetrahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Calcium citrate ...	1305018-01	21249	40	20130528
Caelo	Calcium citrate ...	13391203	21486	40	20131205
Euro OTC	Calcium citrate ...	1509039	21931	40	20151013*
Euro OTC	Calcium citrate ...	1509039-01	22255	40	20151013
Euro OTC	Calcium citrate ...	1701001	22995	40	20170124*

Validation samples

A total of 280 317 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 *Calcium citrate tetrahydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1618 batches from further 372 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 [†].

- 280 spectra of 8 reference samples from the substance/substance group *Calcium citrate tetrahydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium citrate tetrahydrate	13391203	21320	40
Euro OTC	Calcium citrate tetrahydrate	1509039	21931 [†]	20
Euro OTC	Calcium citrate tetrahydrate	1509039-01	22255 [†]	20
Euro OTC	Calcium citrate tetrahydrate	1606001	22681	40
Euro OTC	Calcium citrate tetrahydrate	1707025	23606	40
Caelo	Calcium citrate tetrahydrate	171768	23651	40
Euro OTC	Calcium citrate tetrahydrate	1803031	24077	40
Caelo	Calcium citrate tetrahydrate	181608	24230	40

- 126 612 spectra from a total of 2781 batches from further 781 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.

- 169 spectra from 78 *Apo-Ident* customers from 84 batches from the substance/substance group *Calcium citrate tetrahydrate*.

Supplier	Substance	Batch	Spectra
Caelo	Calcium citrate tetrahydrate	11168813	1
Caelo	Calcium citrate tetrahydrate	11349304	2
Caelo	Calcium citrate tetrahydrate	11349309	2
Caelo	Calcium citrate tetrahydrate	11349301	1
Caelo	Calcium citrate tetrahydrate	11349313	2
Caelo	Calcium citrate tetrahydrate	11168803	1
Caelo	Calcium citrate tetrahydrate	11168806	3
Euro OTC	Calcium citrate tetrahydrate	1009030-01	1
Euro OTC	Calcium citrate tetrahydrate	1207006-01	3
Caelo	Calcium citrate tetrahydrate	11349320	1
Caelo	Calcium citrate tetrahydrate	11349318	3
Caelo	Calcium citrate tetrahydrate	11349325	2
Caelo	Calcium citrate tetrahydrate	12310402	2
Caelo	Calcium citrate tetrahydrate		2
Fagron	Calcium citrate tetrahydrate	13d16-n06	1
Caelo	Calcium citrate tetrahydrate	12310403	3
Caelo	Calcium citrate tetrahydrate	12310407	2
Caelo	Calcium citrate tetrahydrate	1168813	1
Caelo	Calcium citrate tetrahydrate	19061315	1
Caelo	Calcium citrate tetrahydrate	71356168	1
Euro OTC	Calcium citrate tetrahydrate	1211007-01	2
Caelo	Calcium citrate tetrahydrate	12310406	5
Caelo	Calcium citrate tetrahydrate	12310401	1
Sanacorp	Calcium citrate tetrahydrate	1211007-01	1
Euro OTC	Calcium citrate tetrahydrate	1058904	1
EuRho/Jenne	Calcium citrate tetrahydrate	1211007-01	1
Fagron	Calcium citrate tetrahydrate	13D16-N06	1
Caelo	Calcium citrate tetrahydrate	12310401	1
Caelo	Calcium citrate tetrahydrate	1168806	1
Euro OTC	Calcium citrate tetrahydrate	1305018-01	3
Caelo	Calcium citrate tetrahydrate	12310413	4
Caelo	Calcium citrate tetrahydrate	12310411	2
Caelo	Calcium citrate tetrahydrate	92457399	1
Caelo	Calcium citrate tetrahydrate	12310417	3
Euro OTC	Calcium citrate tetrahydrate	13031204	1
Phönix	Calcium citrate tetrahydrate	1305018-01	1
Caelo	Calcium citrate tetrahydrate	12310418	2
Euro OTC	Calcium citrate tetrahydrate	1305018-02	1
Caelo	Calcium citrate tetrahydrate	133912042x	1
Caelo	Calcium citrate tetrahydrate	13391205	5
Caelo	Calcium citrate tetrahydrate	13391203	4
Caelo	Calcium citrate tetrahydrate	2114M1209	1
Euro OTC	Calcium citrate tetrahydrate	1402003-01	2
Caelo	Calcium citrate tetrahydrate	3512U-01209	1
Alliance Health 23.10.2...	Calcium citrate tetrahydrate	1402003-01	1
Caelo	Calcium citrate tetrahydrate	14133303	1
Caelo	Calcium citrate tetrahydrate	16021502	1
Gehe Kassel	Calcium citrate tetrahydrate	14133307	1
Caelo	Calcium citrate tetrahydrate	1408017-01	1
Euro OTC	Calcium citrate tetrahydrate	140801701	1
Caelo	Calcium citrate tetrahydrate	14133307	1
Euro OTC	Calcium citrate tetrahydrate	3006222	1

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Supplier	Substance	Batch	Spectra
Caelo	Calcium citrate tetrahydrate	14133310	1
Caelo	Calcium citrate tetrahydrate	15177703	7
Caelo	Calcium citrate tetrahydrate	15177701	1
Caelo	Calcium citrate tetrahydrate	92192429	1
Euro OTC	Calcium citrate tetrahydrate	1502012-01	1
ACM	Calcium citrate tetrahydrate	KNC0740J15	1
Fagron	Calcium citrate tetrahydrate	150903901	1
Caelo	Calcium citrate tetrahydrate	15177702	2
EuRho	Calcium citrate tetrahydrate	1502012-02	1
Euro OTC	Calcium citrate tetrahydrate	1408017-01	2
Caelo	Calcium citrate tetrahydrate	1509039-01	1
Noweda	Calcium citrate tetrahydrate	1509039-01	1
Euro OTC	Calcium citrate tetrahydrate	1509039-02	6
Euro OTC	Calcium citrate tetrahydrate	1509039-01	2
Caelo	Calcium citrate tetrahydrate	15375702	3
Euro OTC	Calcium citrate tetrahydrate	15177704	1
Caelo	Calcium citrate tetrahydrate	15375707	1
Caelo	Calcium citrate tetrahydrate	15375712	2
Euro OTC	Calcium citrate tetrahydrate	1502021-02	1
Caelo	Calcium citrate tetrahydrate	15375713	6
Caelo	Calcium citrate tetrahydrate	16056504	4
Caelo	Calcium citrate tetrahydrate	15375703	1
Caelo	Calcium citrate tetrahydrate	16056501	1
Euro OTC	Calcium citrate tetrahydrate	1606001-01	1
Caelo	Calcium citrate tetrahydrate	1509039-02	1
Euro OTC	Calcium citrate tetrahydrate	1606001-02	1
Caelo	Calcium citrate tetrahydrate	1606001-02	1
Euro OTC	Calcium citrate tetrahydrate	1701001-01	1
Caelo	Calcium citrate tetrahydrate	16056505	2
Sanacorp WE: 12.08.17 ...	Calcium citrate tetrahydrate	711105	1
Dr.Lohmann	Calcium citrate tetrahydrate	3042527	1
Euro OTC	Calcium citrate tetrahydrate	1701001-02	1
Caelo	Calcium citrate tetrahydrate	1600565	1
Caelo	Calcium citrate tetrahydrate	16056510	2
Caelo	Calcium citrate tetrahydrate	17176803	4
Noweda	Calcium citrate tetrahydrate	17176803	1
lohmann	Calcium citrate tetrahydrate	3045397	1
Caelo	Calcium citrate tetrahydrate	1716803	1
Euro OTC	Calcium citrate tetrahydrate	1710007-01	1
Caelo	Calcium citrate tetrahydrate	17176808	6
Caelo	Calcium citrate tetrahydrate	17176806	1
Caelo	Calcium citrate tetrahydrate	17176805	1
Caelo	Calcium citrate tetrahydrate	17176812	2
Krieger	Calcium citrate tetrahydrate	17176808	1

- 78 760 spectra from 565 *Apo-Ident* customers from a total of 26 055 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

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

	False positive	True positive	False negative	True negative
Type A	0	196	4	74 296
Type B	0	264	16	126 612
Type C	0	159	10	78 760

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	98.0000 % (> 96.5000 %)
Type B	100.0000 % (> 99.9901 %)	94.2857 % (> 93.2143 %)
Type C	100.0000 % (> 99.8817 %)	94.0828 % (> 92.3077 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21249	22995	3.64	38.28
21486	22995	3.82	34.89
21931	21931	0.00	44.87
22255	21931	1.80	43.46
22995	22995	0.00	40.81

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Calcium gluconate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20871-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Calcium gluconate; Calcii gluconas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Calcium gluconate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium gluconate	12236502	20871	40	1401575
Euro OTC	Calcium gluconate	1304012-01	21283	40	AR-15-FG-008127-01
Caelo	Calcium gluconate	12335829	21312	40	20121121
Euro OTC	Calcium gluconate	1407041-01	21821	40	20140818

Validation samples

A total of 280317 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 *Calcium gluconate*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 *Calcium gluconate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Calcium gluconate	1407041-01	21821 [†]	20
Euro OTC	Calcium gluconate	1606034	22699	40
Caelo	Calcium gluconate	154356	23360	40
Euro OTC	Calcium gluconate	1712007	23873	40
Caelo	Calcium gluconate	181010	24017	40

- 126712 spectra from a total of 2784 batches from further 781 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.

- 104 spectra from 60 *Apo-Ident* customers from 46 batches from the substance/substance group *Calcium gluconate*.

[†]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
Fagron	Calcium gluconate	10G22-N12	1
Euro OTC	Calcium gluconate	1105027-02	3
Finze	Calcium gluconate	917857359	1
Euro OTC	Calcium gluconate	1105027-01	1
Euro OTC	Calcium gluconate	115027-01	1
Euro OTC	Calcium gluconate	20270912-1	1
Euro OTC	Calcium gluconate	513-Q1211	1
Fagron	Calcium gluconate	12D17-N01	1
Euro OTC	Calcium gluconate	1209006-01	6
Eurho/Sns	Calcium gluconate	1209006-01	1
EuRho	Calcium gluconate	1209006-01	4
Caelo	Calcium gluconate	12335813	1
Caelo	Calcium gluconate	12335810	1
Euro OTC	Calcium gluconate	1304012-01	4
EuRho	Calcium gluconate	1304012-01	3
Gatt-Koller / Phoenix	Calcium gluconate	550/03141214	1
Euro/Gehe	Calcium gluconate	1304012-01	1
Caelo	Calcium gluconate	14085405	1
sanacorp	Calcium gluconate	1407041-01	1
Fagron	Calcium gluconate	14D11-B04-294136	1
Berkel AHK	Calcium gluconate	14085407	2
Euro OTC	Calcium gluconate	1407041-01	6
Euro OTC	Calcium gluconate	1304012-02	2
Caelo	Calcium gluconate	14230706	1
Fagron	Calcium gluconate	14D11-B04	1
EuRho	Calcium gluconate	12090006-01	1
Caelo	Calcium gluconate	15126301	1
Caelo	Calcium gluconate	1407041-01	1
Euro OTC	Calcium gluconate	130401202	1
Euro OTC	Calcium gluconate	140704102	1
Euro OTC	Calcium gluconate	140704101	1
Euro OTC	Calcium gluconate	1407041-02	9
Caelo	Calcium gluconate	15324806	1
Fagron	Calcium gluconate	15D13-B98-307445	1
Caelo	Calcium gluconate	1543601	1
Caelo	Calcium gluconate	15324807	1
Phönix	Calcium gluconate	1606034-01	1
Caelo	Calcium gluconate	15435607	2
Caelo	Calcium gluconate	1407041-02	1
Caelo	Calcium gluconate	140704102	1
Caelo	Calcium gluconate	15435601	2
Euro OTC	Calcium gluconate	1606034-01	11
Caelo	Calcium gluconate	1606034	1
Caelo	Calcium gluconate	15435611	1
Caelo	Calcium gluconate	15435620	2
Phönix/Euro	Calcium gluconate	1606034-01	1
Euro OTC	Calcium gluconate	1606034-02	2
Caelo	Calcium gluconate	15435619	1
Caelo	Calcium gluconate	15435622	2
Caelo	Calcium gluconate	1000041-01	1
Caelo	Calcium gluconate	15435613	1
Euro OTC	Calcium gluconate	1602001644	1
Euro OTC	Calcium gluconate	1712007-01	2
Caelo	Calcium gluconate	18101004	1
Caelo	Calcium gluconate	18106202	1
Sidonia	Calcium gluconate	18101004	1
Caelo	Calcium gluconate	18101003	1
Gehe/EuRo	Calcium gluconate	1712007-01	1

- 78 825 spectra from 565 *Apo-Ident* customers from a total of 26 091 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Calcium gluconate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium gluconate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	180	0	126 712
Type C	0	97	7	78 825

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	93.2692 % (> 90.3846 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20871	20871	0.00	54.53
21312	20871	5.29	56.99
21283	21283	0.00	41.74
21821	21283	7.68	39.86

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Calcium glycerophosphate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20352-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Calcium glycerophosphate; Calcii glycerophosphas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Calcium glycerophosphate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium glycerop...	12012417	20771	40	20120131
Fagron	Calcium glycerop...	13I17-N04	21234	40	20131016
Caelo	Calcium glycerop...	13007912	21311	40	20130124
Caelo	Calcium glycerop...	14341007	21969	40	AR-16-FG-005932-01
Fagron	Calcium glycerop...	15B03-B03-305050	21978	40	1706313

Validation samples

A total of 280317 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 *Calcium glycerophosphate*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 *Calcium glycerophosphate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium glycerophosphate	12012411	20679	40
Caelo	Calcium glycerophosphate	12012417	20762	40
Caelo	Calcium glycerophosphate	12012413	20763	40
Caelo	Calcium glycerophosphate	14341007	21969 [†]	20
Fagron	Calcium glycerophosphate	15B03-B03-305050	21978 [†]	20
Caelo	Calcium glycerophosphate	162310	23361	40

- 126692 spectra from a total of 2783 batches from further 781 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.

- 71 spectra from 46 *Apo-Ident* customers from 42 batches from the substance/substance group *Calcium glycerophosphate*.

[†]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
Fagron	Calcium glycerophosphate	11G19-N05	1
Caelo	Calcium glycerophosphate	12012406	1
Fagron	Calcium glycerophosphate	12I18-N06	3
Caelo	Calcium glycerophosphate	12012413	2
Fagron	Calcium glycerophosphate	1216000005	1
Fagron	Calcium glycerophosphate	13A18-N02	5
Fagron	Calcium glycerophosphate	13A18N02	2
Caelo	Calcium glycerophosphate	13007902	1
Caelo	Calcium glycerophosphate	13A18-No2	1
Fagron	Calcium glycerophosphate	1317-N04	2
Caelo	Calcium glycerophosphate	13007912	2
Gatt-Koller/Kwizda	Calcium glycerophosphate	4007/09123812	1
Fagron	Calcium glycerophosphate	1314000019	1
Caelo	Calcium glycerophosphate	13007908	1
Caelo	Calcium glycerophosphate	13007914	1
Fagron	Calcium glycerophosphate	14B10-B02-291642	1
Caelo	Calcium glycerophosphate	14347101	2
Fagron	Calcium glycerophosphate	14B10-B02-296841	4
Caelo	Calcium glycerophosphate	14B10-B02-296841	1
Fagron	Calcium glycerophosphate	14B10B02	1
Fagron	Calcium glycerophosphate	5212M-01212	1
Fagron	Calcium glycerophosphate	15B03B03	1
Fagron	Calcium glycerophosphate	14B10-B02	1
Caelo	Calcium glycerophosphate	14341007	5
Caelo	Calcium glycerophosphate	15B03-B03-305050	1
Caelo	Calcium glycerophosphate	15B03B03305050	1
Fagron	Calcium glycerophosphate	15B03-B03	1
Caelo	Calcium glycerophosphate	14341010	1
Fagron	Calcium glycerophosphate	15B03-B03-305050	2
Fagron	Calcium glycerophosphate	3115A-01212	1
Caelo	Calcium glycerophosphate	14341009	1
Caelo	Calcium glycerophosphate	14341013	1
Caelo	Calcium glycerophosphate	14341015	1
Caelo	Calcium glycerophosphate	16231004	2
Caelo	Calcium glycerophosphate	16231001	3
Caelo	Calcium glycerophosphate	162310	1
Caelo	Calcium glycerophosphate	16231006	3
Caelo	Calcium glycerophosphate	16231005	1
Caelo	Calcium glycerophosphate	16231007	2
Caelo	Calcium glycerophosphate	16231010	1
Caelo	Calcium glycerophosphate	17359101	2
Sidonia	Calcium glycerophosphate	17250703	1
Cealo/Sanacorp	Calcium glycerophosphate	17359101	1
Caelo	Calcium glycerophosphate	180918A	1
Caelo	Calcium glycerophosphate	17359106	1

- 78 858 spectra from 565 *Apo-Ident* customers from a total of 26 095 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	200	0	126 692
Type C	0	54	17	78 858

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8817 %)	76.0563 % (> 71.8310 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20771	21969	22.39	34.80
21969	21969	0.00	35.92
21978	21978	0.00	34.07
21234	21969	9.38	39.33
21311	21969	5.58	38.65

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Calcium lactate pentahydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20745-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium lactate pentahydrate; Calcii lactas pentahydricus

Special notes

When selecting the *Calcium lactate pentahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Calcium lactate pentahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Calcium lactate ...	12E10-N03	20745	40	20120704
Fagron	Calcium lactate ...	12I12-N06	21232	40	AR-15-FG-007939-01
Caelo	Calcium lactate ...	15101401	21909	40	20150407
Caelo	Calcium lactate ...	15101405	22263	40	20150407
Caelo	Calcium lactate ...	161313	22445	40	20160513*

Validation samples

A total of 280317 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 *Calcium lactate pentahydrate*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 6 reference samples from the substance/substance group *Calcium lactate pentahydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium lactate pentahydrate	15101401	21909 [†]	20
Caelo	Calcium lactate pentahydrate	15101405	22263 [†]	20
Caelo	Calcium lactate pentahydrate	161313	22445 [†]	20
Fagron	Calcium lactate pentahydrate	14H01-B05-323830	23566	40
Caelo	Calcium lactate pentahydrate	171377	23642	40
Caelo	Calcium lactate pentahydrate	180734	24035	40

- 126712 spectra from a total of 2783 batches from further 781 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*.

- 49 spectra from 18 *Apo-Ident* customers from 29 batches from the substance/substance group *Calcium lactate pentahydrate*.

Supplier	Substance	Batch	Spectra
Caelo	Calcium lactate pentahydrate	12E10-N03	1
Caelo	Calcium lactate pentahydrate	11369610	1
Shop	Calcium lactate pentahydrate	1111001829	1
Caelo	Calcium lactate pentahydrate	12C15-N02	1
Fagron	Calcium lactate pentahydrate	12C15-N02	1
Caelo	Calcium lactate pentahydrate	11369618	1
Caelo	Calcium lactate pentahydrate	11369614	2
Fagron	Calcium lactate pentahydrate	12I12-N01	1
Fagron	Calcium lactate pentahydrate	12/12-N06	1
Caelo	Calcium lactate pentahydrate	13080802	2
Caelo	Calcium lactate pentahydrate	13080804	2
Caelo	Calcium lactate pentahydrate	13080805	2
Fagron	Calcium lactate pentahydrate	13L18B04	1
Fagron	Calcium lactate pentahydrate	12I12-N06	2
Fagron	Calcium lactate pentahydrate	13L18-B04-295541	3
Caelo	Calcium lactate pentahydrate	11369606	1
Fagron	Calcium lactate pentahydrate	14H01-B05	1
Caelo	Calcium lactate pentahydrate	14H01B05300502	1
phönix	Calcium lactate pentahydrate	15101411	1
Caelo	Calcium lactate pentahydrate	15227804	2
Caelo	Calcium lactate pentahydrate	15101409	1
Caelo	Calcium lactate pentahydrate	15101411	2
Caelo	Calcium lactate pentahydrate	16131307	1
Phönix	Calcium lactate pentahydrate	14H01-B05	1
Caelo	Calcium lactate pentahydrate	15101412	3
Caelo	Calcium lactate pentahydrate	16131302	1
Caelo	Calcium lactate pentahydrate	16131312	1
Caelo	Calcium lactate pentahydrate	16333106	3
Caelo	Calcium lactate pentahydrate	16333111	4
Caelo	Calcium lactate pentahydrate	17137707	2
Caelo	Calcium lactate pentahydrate	17355503	1
Fagron	Calcium lactate pentahydrate	17J18-B01-347174	1

- 78 880 spectra from 565 *Apo-Ident* customers from a total of 26 108 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Calcium lactate pentahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium lactate pentahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	180	0	126 712
Type C	0	49	0	78 880

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 87.7551 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20745	22445	4.82	37.94
22263	22445	4.67	38.36
21232	21232	0.00	36.61
21909	22445	4.98	38.22
22445	22445	0.00	38.55

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Calcium orotate dihydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20418-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Calcium orotate dihydrate; Calcii oroticum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Calcium orotate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Calcium orotate ...	12L04-N07	20824	40	20121207
Fagron	Calcium orotate ...	13J23-N05	21227	40	20131111
Euro OTC	Calcium orotate ...	1401006-01	21245	40	1412540
Euro OTC	Calcium orotate ...	1603003	22520	40	20160329*
Euro OTC	Calcium orotate ...	1603003	24164	40	20180615*

Validation samples

A total of 280317 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 *Calcium orotate dihydrate*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1619 batches from further 372 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 *Calcium orotate dihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Calcium orotate dihydrate	1009035-01	20814	40
Euro OTC	Calcium orotate dihydrate	1411003	22519	40
Fagron	Calcium orotate dihydrate	16F13-B04-324144	23574	40

- 126772 spectra from a total of 2786 batches from further 781 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 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Calcium orotate dihydrate*.

*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
Euro OTC	Calcium orotate dihydrate	1203037-01	2
Euro OTC	Calcium orotate dihydrate	1401006-01	1

- 78 926 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Calcium orotate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium orotate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	79	41	126 772
Type C	0	3	0	78 926

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	65.8333 % (> 63.3333 %)
Type C	100.0000 % (> 99.8821 %)	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
22520	22520	0.00	88.95
24164	24164	0.00	89.34
20824	21245	1.26	61.73
21227	21245	3.01	61.50
21245	21245	0.00	62.08

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Calcium pantothenate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20395-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium pantothenate; Calcii panthothenicum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Calcium pantothenate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Calcium pantothe...	13H28-N11	21233	40	20130916
Euro OTC	Calcium pantothe...	1305034-01	21243	40	20130617
Caelo	Calcium pantothe...	14208012	21765	40	20140722
Euro OTC	Calcium pantothe...	1509024	21901	40	20151005*
Euro OTC	Calcium pantothe...	1603042	22551	40	20160429*

continued on the next page

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Calcium pantothe...	1607023	22691	40	20160809*
Euro OTC	Calcium pantothe...	1702018	23153	40	20170330*
Euro OTC	Calcium pantothe...	1711003	23890	40	20171123*

Validation samples

A total of 280 317 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 *Calcium pantothenate*. These samples are listed above in the [calibration samples](#) section.
- 74 176 spectra from a total of 1615 batches from further 372 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 7 reference samples from the substance/substance group *Calcium pantothenate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium pantothenate	14208012	21765 [†]	20
Euro OTC	Calcium pantothenate	1509024	21901 [†]	20
Caelo	Calcium pantothenate	162516	23363	40
Caelo	Calcium pantothenate	15344217	23717	40
Caelo	Calcium pantothenate	173352	24045	40
Euro OTC	Calcium pantothenate	1803014	24081	40
Euro OTC	Calcium pantothenate	1809014	24312	40

- 126 652 spectra from a total of 2782 batches from further 781 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.

- 65 spectra from 36 *Apo-Ident* customers from 40 batches from the substance/substance group *Calcium pantothenate*.

Supplier	Substance	Batch	Spectra
Fagron	Calcium pantothenate	1111110405	1
Caelo	Calcium pantothenate	11105731	1
Caelo	Calcium pantothenate	1013Q-03022	1
Gehe	Calcium pantothenate	1004024-01	1
Euro OTC	Calcium pantothenate	1209022-01	1
Caelo	Calcium pantothenate	12236622	1
Euro OTC	Calcium pantothenate	1111025-01	1
Euro OTC	Calcium pantothenate	1209022-02pzn	1
Fagron	Calcium pantothenate	1111025-01	1
Caelo	Calcium pantothenate	12340808	3
Caelo	Calcium pantothenate	27111303	1
Euro OTC	Calcium pantothenate	1305034-01	4
Caelo	Calcium pantothenate	12340819	2
Caelo	Calcium pantothenate	12340809	1
Euro OTC	Calcium pantothenate	130503401	2
Caelo	Calcium pantothenate	12340832	1
Euro OTC	Calcium pantothenate	1312027-01	3
Euro OTC	Calcium pantothenate	17021401	1
Caelo	Calcium pantothenate	8041407	1
Fagron	Calcium pantothenate	12F19-N07	1
Caelo	Calcium pantothenate	12340846	1
Euro OTC	Calcium pantothenate	1209022-02	1
Fagron	Calcium pantothenate	13H28-N11	1
Euro OTC	Calcium pantothenate	5121405	1
Caelo	Calcium pantothenate	12340859	1
Euro OTC	Calcium pantothenate	10021505	1
Caelo	Calcium pantothenate	14208004	1
Noweda	Calcium pantothenate	14208012	1
Fagron	Calcium pantothenate	14G02-B10-297373	1
Euro OTC	Calcium pantothenate	1410011-01	1
Euro OTC	Calcium pantothenate	1410011-02	3
Caelo	Calcium pantothenate	1410011-02	1
Caelo	Calcium pantothenate	1410011-01	1
Euroo/Anzag	Calcium pantothenate	1509024-01	2
Euro OTC	Calcium pantothenate	1509024-01	3
Euro OTC	Calcium pantothenate	1603042-01	3
Caelo	Calcium pantothenate	15344207	1
Caelo	Calcium pantothenate	1509024-01	1
Caelo	Calcium pantothenate	1607023-01	2
Euro OTC	Calcium pantothenate	18111707	1
Euro OTC	Calcium pantothenate	1711003-01	1
Euro OTC	Calcium pantothenate	1803014-01	3
Caelo	Calcium pantothenate	16251608	1
Anzag/Anzag 26.07.18	Calcium pantothenate	1803017-01	1
Caelo	Calcium pantothenate	17335208	2

- 78 864 spectra from 565 *Apo-Ident* customers from a total of 26 098 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Calcium pantothenate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium pantothenate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 176
Type B	0	240	0	126 652
Type C	0	63	2	78 864

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.8817 %)	96.9231 % (> 92.3077 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
22551	22551	0.00	13.56
21233	23153	6.29	21.76
21243	23153	9.96	23.48
21765	23153	9.61	23.85
23153	23153	0.00	21.01
23890	23890	0.00	20.22
22691	22691	0.00	13.98
21901	21901	0.00	19.78

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Camphor**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20028-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Camphor; Camphora

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Camphor	1406029-01	21599	40	20140708
Fagron	Camphor	14E19-B07-300365	22256	40	20140527
Caelo	Camphor	15316801	22279	40	20151029
Caelo	Camphor	162354	23065	40	20160809*
Caelo	Camphor	170043	23310	40	20170220*

Validation samples

A total of 280317 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 *Camphor*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 7 reference samples from the substance/substance group *Camphor*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Camphor	1406029-01	21599 [†]	20
Fagron	Camphor	14E19-B07-300365	22256 [†]	20
Caelo	Camphor	15316801	22279 [†]	20
Caelo	Camphor	16209309	23408	40
Fagron	Camphor	16E23-B08-336937	23589	40
Caelo	Camphor	172883	23804	40
Caelo	Camphor	180198	24013	40

- 126672 spectra from a total of 2782 batches from further 781 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*.

- 420 spectra from 223 *Apo-Ident* customers from 188 batches from the substance/substance group *Camphor*.

Supplier	Substance	Batch	Spectra
Euro OTC	Camphor	1101029-02	1
Caelo	Camphor	11286905	2
Fagron	Camphor	12B14-N09	1
Caesar & Loretz GmbH, 4...	Camphor	11032035	1
Noweda	Camphor	1202021-01	1
Fagron	Camphor	11H30-N15	1
Caelo	Camphor	3091203	1
Euro OTC	Camphor	1202021-01	2
Caelo	Camphor	2811Q-01221	1
Caelo	Camphor	11032035	2
Caelo	Camphor	11032023	1
Euro OTC	Camphor	1202021	1
EuRho	Camphor	2111E-01219	1
Fagron	Camphor	12D23-N03	1
Euro OTC	Camphor	1202021-02	1
Fagron	Camphor	11K23-N04	1
Euro OTC	Camphor	113Q-01221	1
Caelo	Camphor	11074509	1
Caelo	Camphor	11286909	2
Caelo	Camphor	12054105	1
Caelo	Camphor	12054107	4
Euro OTC	Camphor	121003001	1
Euro OTC	Camphor	1210030-01	6
Caelo	Camphor	1210030-01	1
Caelo	Camphor	12054124	2
Gehe	Camphor	1210030-01	1
Caelo	Camphor	120564113	1
Caelo	Camphor	12054113	1
Sanacorp	Camphor	11032035	1
Caelo	Camphor	1210030-02	1
Euro OTC	Camphor	1210030-02	4
Caelo	Camphor	12054141	3
Caelo	Camphor	12344905	2
Caelo	Camphor	12054142	6
xxx	Camphor	709E-01221	1
Caelo	Camphor	12228205	1
Caelo	Camphor	2344905	1
Caelo	Camphor	12228206	1
Klenk	Camphor	444A100826	1
Euro OTC	Camphor	1303013-01	4
Fagron	Camphor	690442	1
Fagron	Camphor	12G02-N09	1
Caelo	Camphor	13108106	2
Caelo	Camphor	11286910	1
Euro OTC	Camphor	1101029-02/Ch241011	1
Phönix	Camphor	1202021-02	1
Bombastus	Camphor	1303013-01	1
Caelo	Camphor	4101303	1
Euro OTC	Camphor	1303013-02	8
Sanacorp	Camphor	444A130115	1
euroct/gehe	Camphor	1303013-02	1
Caelo	Camphor	12054151	2
Caelo	Camphor	12054149	7
Caelo	Camphor	12054114	2
Euro OTC	Camphor	2803020-01	2

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Supplier	Substance	Batch	Spectra
Sanacorp	Camphor	12054149	1
Galke	Camphor	23624	1
EuRho	Camphor	1303013-02	2
Caelo	Camphor	13205501	2
Caelo	Camphor	13195304	1
Caelo	Camphor	12054143	1
Caelo	Camphor	13195301	2
Euro OTC	Camphor	130313-02	1
Post-Apotheke 22.01.2013	Camphor	11032012	1
Caelo	Camphor	12243701	1
Caeöo	Camphor	12054149	1
Fagron	Camphor	13H23-B04-288376	1
Caelo	Camphor	713A-01221	1
Caelo	Camphor	13195311	2
Caelo	Camphor	13205512	2
Caelo	Camphor	13205511	3
Caelo	Camphor	13205502	1
Caelo	Camphor	13195314	8
Caesar/Noweda	Camphor	1032	1
Caelo	Camphor	25041401	1
Caelo	Camphor	12061411	1
	Camphor	12344909	1
Fagron	Camphor	13H23-B40-291888	1
Cealo/ Noweda	Camphor	13108116	1
Fagron	Camphor	13K28-B04	2
Euro OTC	Camphor	1309019-03	1
Fagron	Camphor	13H23-B40-294116	1
Fagron	Camphor	8082014A	1
Caelo	Camphor	13195316	6
Fagron	Camphor	13h23-b40-294116	1
Caelo	Camphor	13205522	3
Euro OTC	Camphor	1309019-02	1
Caelo	Camphor	13195318	1
Caelo	Camphor	13108118	2
Fagron	Camphor	825653	1
Caelo	Camphor	14224303	3
Fagron	Camphor	13H23-B40-296252	1
Caelo	Camphor	13K28-04-294937	1
Klenk	Camphor	444A140526	3
Fagron	Camphor	14G23-B04-296868	1
Fagron	Camphor	14G23-B04-299202	2
Sanacorp	Camphor	14224303	1
Fagron	Camphor	14G23-B04	2
Caelo	Camphor	914E-01221	1
Caelo	Camphor	13195322	7
Caelo	Camphor	14202801	1
phönix	Camphor	14202801	1
Fagron	Camphor	13K28-B04-294937	1
Caelo	Camphor	4031503	1
Phönix	Camphor	13K28-B04	1
Caelo	Camphor		2
Phönix Gotha	Camphor	14202801	1
Caesar/Noweda	Camphor	13195328	1
Fagron	Camphor	14G23-B04-301878	2
Caelo	Camphor	444A140526	1
Euro OTC	Camphor	821509	1
Caelo	Camphor	14202807	2
Caelo	Camphor	13195326	3
Caelo	Camphor	14310703	1
Caelo	Camphor	15097803	2

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Supplier	Substance	Batch	Spectra
Caelo	Camphor	14224304	1
Fagron	Camphor	13K28B04294933	1
Fagron	Camphor	14G23-B04-301879	1
Calo/AHD	Camphor	15086803	1
Fagron	Camphor	15097801	1
Caelo	Camphor	13195323	1
Caelo	Camphor	15120901	2
Caelo	Camphor	15086806	1
Caelo	Camphor	1412023-01	3
Caelo	Camphor	15062702	3
Caelo	Camphor	15097802	2
Caelo	Camphor	15086801	1
Euro OTC	Camphor	1412023-01	1
Caelo	Camphor	14310705	14
Caelo	Camphor	15316801	4
Euro OTC	Camphor	1406029-01	1
Caelo	Camphor	315E-01221	1
Fagron	Camphor	1309019-02	1
Caelo	Camphor	15316807	6
Klenk	Camphor	444A150721	2
Caelo	Camphor	14310709	3
Euro OTC	Camphor	1406029-02	1
Caelo	Camphor	4444A150721	1
Caelo	Camphor	15320604	3
Phoenix	Camphor	15316811	1
Caelo	Camphor	15316806	2
Caelo	Camphor	15316811	6
Caelo	Camphor	13205517	1
Caelo	Camphor	14310109	1
Caelo	Camphor	1410710	1
Caelo	Camphor	14310713	8
Sanacorp	Camphor	14310709	1
Caelo	Camphor	15397705	1
Fagron	Camphor	13K28-B04-289340	1
Caelo	Camphor	15316819	6
Fagron	Camphor	15/18-B11-321658	1
Caelo	Camphor	15316815	4
Caelo	Camphor	15316812	1
Caelo	Camphor	150622C	1
Caelo	Camphor	140918C	1
Caesar&Loretz	Camphor	14310719	1
Camphor & Allied Produc...	Camphor	16209302	1
Caelo	Camphor	16209301	8
Caelo	Camphor	5315I-01221	1
Caelo	Camphor	15120902	1
Klenk	Camphor	444A160817	5
Camphor & Allied Produc...	Camphor	1406029-01	1
Caelo	Camphor	15397704	4
Caelo	Camphor	16209304	2
Caelo	Camphor	14310718	4
Caelo	Camphor	15384201	1
Caelo	Camphor	15397701	1
Caelo	Camphor	16209305	4
Caeolo/Phönix	Camphor	16209305	1
Euro/Noweda	Camphor	15320604	1
Caelo	Camphor	14310722	2
Caesar	Camphor	1406029-02	1
Caelo	Camphor	16209309	8
Caelo	Camphor	16209306	1
Sanacorp	Camphor	14310720	2

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Supplier	Substance	Batch	Spectra
phönix	Camphor	444a160817	1
Caelo	Camphor	16235404	1
Caelo	Camphor	14310715	1
Caelo	Camphor	17004301	10
Gehe	Camphor	16209305	1
Caelo	Camphor	15316823	2
Caelo	Camphor	16209310	1
Gehe	Camphor	16235404	1
Caelo	Camphor	14310710	1
Caelo	Camphor	15316805	1
euro/ Sanacorp	Camphor	17050602	1
GEHE	Camphor	16235408	1
Caelo	Camphor	17004304	1
Phoenix	Camphor	16235405	1
Caelo	Camphor	16235408	1
Caelo	Camphor	17004302	2
Caelo	Camphor	17050606	2
Caelo	Camphor	17050602	1
Sanacorp	Camphor	17004306	1
Caelo	Camphor	13111707	1
Caelo	Camphor	13111708	1
Caelo	Camphor	17004306	5
Gehe	Camphor	17134702	1
Caelo	Camphor	17050605	9
Fagron	Camphor	27011	1
Euro OTC	Camphor	16209304	1
Caelo	Camphor	1531607	1
Caelo	Camphor	17134703	1
Caelo	Camphor	17324104	2
Caelo	Camphor	17050605/1140418	1
Caelo	Camphor	7061802	1
Sanacorp	Camphor	18019802	1
Caelo	Camphor	7071801	1
Caelo	Camphor	17288301	3
Caelo	Camphor	17288305	1
Caelo	Camphor	12091805	1
Caelo	Camphor	18019802	3
Caelo	Camphor	12091808	1
Caelo	Camphor	18019803	2
Caelo	Camphor	18198003	1
Fagron	Camphor	18066404	1
Nachtestung-Verlängerung	Camphor	242/17	1
Caelo	Camphor	18066404	1
Caelo	Camphor	18019806	2
Kehr	Camphor	18066404	1
Caelo	Camphor	6021901	1

- 78 509 spectra from 565 *Apo-Ident* customers from a total of 25 953 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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* can clearly be 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* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	220	0	126 672
Type C	0	391	29	78 509

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.8817 %)	93.0952 % (> 92.3810 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21599	23065	8.25	53.70
22279	23065	7.30	53.76
23065	23065	0.00	53.44
23310	23310	0.00	52.73
22256	23310	18.29	51.77

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Cannabidiol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22416-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Cannabidiol

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Cannabidiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22412	40	1316Q-07806
THC-Pharma GmbH	Cannabidiol	CBD-API17-003	23398	40	20170609
THC-Pharma GmbH	Cannabidiol	CBD-API16-003	23464	40	2017B-03911
THC-Pharma GmbH	Cannabidiol	CBD-API1801	23929	40	20180209
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22412SI	40	1316Q-07806

Validation samples

A total of 280317 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 *Cannabidiol*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1619 batches from further 372 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 [†].

- 791 spectra of 17 reference samples from the substance/substance group *Cannabidiol*.

Supplier	Substance	Batch	Sample ID	Spectra
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22412 [†]	20
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22413	60
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22414	60
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22415	60
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22416	60
THC-Pharma GmbH	Cannabidiol	CBD-API17-003	23399	40
THC-Pharma GmbH	Cannabidiol	CBD-API16-004	23465	40
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22412SI [†]	20
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22413SI	60
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22414SI	60
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22415SI	60
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22416SI	60
THC-Pharma GmbH	Cannabidiol	CBD-API17-003	23398SI	40
THC-Pharma GmbH	Cannabidiol	CBD-API17-003	23399SI	31
THC-Pharma GmbH	Cannabidiol	CBD-API16-003	23464SI	40
THC-Pharma GmbH	Cannabidiol	CBD-API16-004	23465SI	40
THC-Pharma GmbH	Cannabidiol	CBD-API1801	23929SI	40

- 126101 spectra from a total of 2784 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the

[†]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.

- 137 spectra from 13 *Apo-Ident* customers from 31 batches from the substance/substance group *Cannabidiol*.

Supplier	Substance	Batch	Spectra
THC-Pharm	Cannabidiol		12
Caelo	Cannabidiol	110216-02	3
THC-Pharm	Cannabidiol	cbd-adi17-002	1
THC	Cannabidiol	CBD-API17-002	2
THC Pharm GmbH / THC Ph...	Cannabidiol	CBD-API17-005	1
THC-Pharma	Cannabidiol	CBD-API17-003	1
THC	Cannabidiol	CBD-API17-003	1
THC Pharm GmbH	Cannabidiol	CBD-API17-005	3
THC-Pharm	Cannabidiol	CBDAP/17-003	3
THC Pharma	Cannabidiol	CBD-API17-004	3
THC/Gehe	Cannabidiol	CBD-API17-005	1
THC Pharm	Cannabidiol	CBD-API16-004	1
THC	Cannabidiol	CBD-API17-004	4
THC-Pharm	Cannabidiol	CBD-API17-005	1
THC Pharm	Cannabidiol	CBD-API17-004	1
THC-Pharm	Cannabidiol	CBD-API17-004	1
Caelo	Cannabidiol	CBD-API17-006	2
THC Pharma (direkt)	Cannabidiol	CBD-API17-006	1
THC Pharm GmbH	Cannabidiol	CBD-API17-006	1
THC	Cannabidiol	CBD-API17-006	2
THC Pharm GmbH	Cannabidiol	CBDAP1707	1
THC Pharma (direkt)	Cannabidiol	CBDAP1708	1
THC Pharma (direkt)	Cannabidiol	CBDAP1707	1
THC-Pharma	Cannabidiol	CBDAP1708	1
THC-Pharma	Cannabidiol	CBDAP/1708	1
THC/ Direkt	Cannabidiol	CBDAP1706	1
Caelo	Cannabidiol	CBDAP1801	2
THC Pharm GmbH	Cannabidiol	CBDAP1801	2
THC Pharma (direkt)	Cannabidiol	CBDAP1801	1
THC Pharm GmbH	Cannabidiol		9
THC Pharma (direkt)	Cannabidiol		2
THC Pharm	Cannabidiol	H150218-1	1
THC Pharm	Cannabidiol		13
THC-Pharma	Cannabidiol		8
THC Pharm GmbH	Cannabidiol	CBDAP1802	1
Bombastus	Cannabidiol		1
Sanacorp	Cannabidiol		6
Sanacorp	Cannabidiol	CBDAP1804	3
THC-Pharma	Cannabidiol	CBDAP1804	1
THC Pharm GmbH	Cannabidiol	CBDAP1804	1
THC Pharma	Cannabidiol	CBDAP1804	1
THC Pharm/ Sanacorp	Cannabidiol		16
THC Pharm	Cannabidiol	CBDAP1804	1
THC Pharma	Cannabidiol		3
THC Pharma	Cannabidiol	CBDAP1802	1
THC-Pharma	Cannabidiol	CBDAP1802	2
Apocare	Cannabidiol	ACPK911004	9

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Supplier	Substance	Batch	Spectra
THC	Cannabidiol		1
Apocare	Cannabidiol	ACPK312001	1

- 78 792 spectra from 565 *Apo-Ident* customers from a total of 26 106 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Cannabidiol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cannabidiol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	790	1	126 101
Type C	0	130	7	78 792

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	99.8736 % (> 99.4943 %)
Type C	100.0000 % (> 99.8817 %)	94.8905 % (> 92.7007 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
22412	22412	0.00	79.18
23398	22412	8.93	80.75
23464	23464	0.00	80.75
23929	22412	15.47	81.23

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Capsaicin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20854-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Capsaicin; Capsaicinoida

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Capsaicin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Capsaicin	13D12-N01	20854	40	1411392
Fagron	Capsaicin	13J07-N07	21340	40	AR-15-FG-007151-01
Euro OTC	Capsaicin	1703023	23145	40	20170407*
Euro OTC	Capsaicin	1811009	24331	40	20181207*

Validation samples

A total of 280317 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 *Capsaicin*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 *Capsaicin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Capsaicin	118066-04	21638	60
Euro OTC	Capsaicin	1603005-01	22930	40
Euro OTC	Capsaicin	1603005-01	22931	40
Euro OTC	Capsaicin	1806013-01	24186	40
Euro OTC	Capsaicin	1812015	24457	40

- 126672 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 20 spectra from 11 *Apo-Ident* customers from 6 batches from the substance/substance group *Capsaicin*.

*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
Fagron	Capsaicin	CP-12003	1
Euro OTC	Capsaicin	1401043-02	2
Euro OTC	Capsaicin	1603005-01	13
Euro OTC	Capsaicin	1703023-025346	1
Euro OTC	Capsaicin	1703023-02	1
EuRho	Capsaicin	1703023-02	1
Euro OTC	Capsaicin	1806013-01	1

- 78 909 spectra from 565 *Apo-Ident* customers from a total of 26 131 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Capsaicin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Capsaicin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	220	0	126 672
Type C	0	19	1	78 909

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.8817 %)	95.0000 % (> 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
20854	20854	0.00	15.88
21340	21340	0.00	19.16
24331	24331	0.00	23.62
23145	23145	0.00	13.97

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Captopril**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20890-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Captopril; Captoprilum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Captopril*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Captopril	12G25-N08	20890	40	20120814
Caelo	Captopril	12339610	21064	40	1403227
Caelo	Captopril	15189502	21874	40	AR-15-FG-014855-01
Fagron	Captopril	14B26-B01-312221	21921	40	20140317

Validation samples

A total of 280 317 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 *Captopril*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 [†].

- 310 spectra of 8 reference samples from the substance/substance group *Captopril*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Captopril	15189502	21874 [†]	20
Fagron	Captopril	14B26-B01-312221	21921 [†]	20
Caelo	Captopril	170772	23366	40
Fagron	Captopril	17G21-B02-337989	23588	30
Caelo	Captopril	172102	23676	40
Caelo	Captopril	15189502	21874SI	60
Fagron	Captopril	14B26-B01-312221	21921SI	60
Caelo	Captopril	170772	23366SI	40

- 126 582 spectra from a total of 2784 batches from further 781 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*.

- 194 spectra from 78 *Apo-Ident* customers from 76 batches from the substance/substance group *Captopril*.

Supplier	Substance	Batch	Spectra
Fagron	Captopril	12G25-N08	4
Fagron	Captopril	12K-16N04	1
Caelo	Captopril	12F29-N04	1
Fagron	Captopril	12K16-N04	1
Herstellung	Captopril	12339607	1
Caelo	Captopril	12339605	4
Caelo	Captopril	12339604	2
Caelo	Captopril	12339610	2
Caelo	Captopril	12339602	1
Caelo	Captopril	12339619	1
Phonix	Captopril	14B26-B01	1
Fagron	Captopril	14B26-B01-291555	3
Caelo/Sanacorp	Captopril	12339617	1
Caelo	Captopril	12339616	2
Caelo	Captopril	12339617	1
Fagron	Captopril	14B26-B01	6
Fagron	Captopril	14B26-B01-291557	5
Fagron	Captopril	14196902	1
Caelo	Captopril	14196903	2
Caelo	Captopril	14196905	3
Caelo	Captopril	14196904	8
Sonnenberg-Apotheke	Captopril	14B26-B01-291557	2
Fagron	Captopril	14B26-B012911557	1
Fagron	Captopril	14B26-W0129-1557	1
Fagron	Captopril	14B26-B01-291556	1
Caelo	Captopril	14B26-B01-291555	1
Caelo	Captopril	14B26-B01-291557	1
Caelo	Captopril	14196901	1
Fagron	Captopril	14B26-B01302338	1
Caelo	Captopril	15189501	6
Caelo	Captopril	15189502	1
Fagron	Captopril	14B26B01	1
Fagron	Captopril	14B26-B01-310127	2
Fagron	Captopril	14B26-B01-302338	2
Caelo	Captopril	14B26-B01-310127	1
Caelo	Captopril	5102-14-042	1
Fagron	Captopril	EC140101	1
Fagron	Captopril	14B26-B01-310127	2
Fagron	Captopril	14B26-B01-314460	1
Caelo	Captopril	14B26-B01-310127	1
Caelo	Captopril	15189507	3
Fagron	Captopril	80616-6	1
Caelo	Captopril	15189503	1
Fagron	Captopril	14B26-B40-318894	5
Fagron	Captopril	14B26-B01-316257	2
Fagron	Captopril	14B26-B01-312221	1
Fagron	Captopril	14B26-B40-320183	5
Caelo	Captopril	15189511	4
Hedinger	Captopril	14B26-B40	2
Fagron	Captopril	14B26-B40-321319	4
Caelo	Captopril	15189514	6
Caelo	Captopril	15189510	2
Fagron	Captopril	700766	1
Euro OTC	Captopril	14B26-B40-320183	1
Changzhou Pharmaceutical	Captopril	14B26-B40-321319	1
Fagron	Captopril	14B26-B01-302337	1
Caelo	Captopril	15189509	2

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Supplier	Substance	Batch	Spectra
Euroct/Gehe	Captopril	14B26-B40-320183	1
Caelo	Captopril	15189512	4
Caelo	Captopril	14B26-B40	1
Caelo	Captopril	14B26-B40-323267	1
Fagron	Captopril	14B26-B40-323267	1
Caelo	Captopril	15189515	1
Caelo	Captopril	15189517	3
Caelo	Captopril	15189521	5
Fagron	Captopril	14B26-B40-325275	2
Caelo	Captopril	14B26-B40-320183	1
Caelo	Captopril	15189519	2
Caelo	Captopril	14B26-B40-325275	2
Caelo	Captopril	16B26-B01310127	1
Caelo	Captopril	15189525	1
Caelo	Captopril	15189524	2
Caelo	Captopril	1519521	1
Caelo	Captopril	17077201	2
Caelo	Captopril	17077205	1
Caelo	Captopril	17077209	6
Caelo	Captopril	17077202	2
Caelo	Captopril	17077208	6
GEHE	Captopril	17210203	1
GEHE	Captopril	17077209	1
Fagron	Captopril	17G27-B02-337989	2
Caesar&Loretz	Captopril	17210201	1
Fagron	Captopril	17g27-b02-337989	1
Caelo	Captopril	17077206	1
Caelo	Captopril	17210202	6
Euro OTC	Captopril	17210204	1
Fagron	Captopril	17G27-B02-340798	2
Caelo	Captopril	17G27-B02	2
Caelo	Captopril	17210205	6
Fagron	Captopril	17G27-B02-346203	1
Caelo	Captopril	17210204	1
Caelo	Captopril	18058003	1

- 78 735 spectra from 565 *Apo-Ident* customers from a total of 26 062 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Captopril* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Captopril* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	303	7	126 582
Type C	0	179	15	78 735

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	97.7419 % (> 96.7742 %)
Type C	100.0000 % (> 99.8817 %)	92.2680 % (> 90.7216 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20890	21064	2.05	42.19
21064	21064	0.00	42.03
21874	21874	0.00	43.55
21921	21874	12.46	44.96

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Carbomers 35000 / 50000**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20548-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Carbomers 35000 / 50000

Special notes

When selecting the *Carbomers 35000 / 50000* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Carbomers 35000 / 50000*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Carbomers 35000 ...	13135601	20978	40	1403767
Caelo	Carbomers 35000 ...	13186207	20979	40	1403768
Caelo	Carbomers 35000 ...	14057902	21354	40	20140228
Euro OTC	Carbomers 35000 ...	1311027-02	21561	40	20131205
Euro OTC	Carbomers 35000 ...	1512010	22250	40	20151216*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Carbomers 35000 ...	1604032	22548	40	20160428*
Euro OTC	Carbomers 35000 ...	1607028	22686	40	20160804*
Caelo	Carbomers 35000 ...	162530	22759	40	20161011*
Euro OTC	Carbomers 35000 ...	1610024	22852	40	20161102*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Carbomers 35000 / 50000*. These samples are listed above in the [calibration samples](#) section.
- 74136 spectra from a total of 1614 batches from further 372 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 *Carbomers 35000 / 50000*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Carbomers 35000 / 50000	14057903	21557	60
Euro OTC	Carbomers 35000 / 50000	1311027-02	21561 [†]	20
Euro OTC	Carbomers 35000 / 50000	1512010	22250 [†]	20
Euro OTC	Carbomers 35000 / 50000	1702012	23139	40
Euro OTC	Carbomers 35000 / 50000	1706015	23534	40
Caelo	Carbomers 35000 / 50000	172520	23621	40
Caelo	Carbomers 35000 / 50000	173614	23783	40
Euro OTC	Carbomers 35000 / 50000	1801044	23959	40
Caelo	Carbomers 35000 / 50000	180924	24250	40
Euro OTC	Carbomers 35000 / 50000	1810019	24315	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*.

- 126 512 spectra from a total of 2779 batches from further 781 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.

- 284 spectra from 175 *Apo-Ident* customers from 96 batches from the substance/substance group *Carbomers 35000 / 50000*.

Supplier	Substance	Batch	Spectra
Euro OTC	Carbomers 35000 / 50000	1202020-01	2
Caelo	Carbomers 35000 / 50000	11351618	3
Caelo	Carbomers 35000 / 50000	11351605	2
Caelo	Carbomers 35000 / 50000	11351604	1
Caelo	Carbomers 35000 / 50000	11351623	1
Caelo	Carbomers 35000 / 50000	12274907	7
Caelo	Carbomers 35000 / 50000	11307511	1
Caelo	Carbomers 35000 / 50000	12274908	4
Euro OTC	Carbomers 35000 / 50000	1210037-01	6
Caelo	Carbomers 35000 / 50000	11013605	2
Caelo	Carbomers 35000 / 50000	12274912	4
EuRho	Carbomers 35000 / 50000	1210037-01	1
Caelo	Carbomers 35000 / 50000	12274910	1
Caelo	Carbomers 35000 / 50000	12274916	7
Caelo	Carbomers 35000 / 50000	12274914	3
Hepart AG	Carbomers 35000 / 50000	12274916	1
Caelo	Carbomers 35000 / 50000	2913M1232	1
Sanacorp	Carbomers 35000 / 50000	12274922	1
Caelo	Carbomers 35000 / 50000	12274922	1
Caelo	Carbomers 35000 / 50000	13186207	1
Euro/Sanacorp	Carbomers 35000 / 50000	1305007-01	1
Euro OTC	Carbomers 35000 / 50000	1305007-01	2
Caelo	Carbomers 35000 / 50000	13186205	6
Euro OTC	Carbomers 35000 / 50000	101217279	1
Caelo	Carbomers 35000 / 50000	13186201	2
Caelo	Carbomers 35000 / 50000	13194503	7
Caelo	Carbomers 35000 / 50000	13194507	4
Gehe	Carbomers 35000 / 50000	13194505	1
Caelo	Carbomers 35000 / 50000	13194505	2
Sanacorp	Carbomers 35000 / 50000	6/AKD13	1
Caelo	Carbomers 35000 / 50000	28111310	1
Caelo	Carbomers 35000 / 50000	13186203	3
Caelo	Carbomers 35000 / 50000	13194501	5
Fagron	Carbomers 35000 / 50000	13194503	1
Caelo	Carbomers 35000 / 50000	13194511	1
Caelo	Carbomers 35000 / 50000	14016208	7
Euro OTC	Carbomers 35000 / 50000	4311027-01	1
Caelo	Carbomers 35000 / 50000	13194512	1
Euro OTC	Carbomers 35000 / 50000	1311027-01	3
Euro OTC	Carbomers 35000 / 50000	12052014A	1
Phoenix 16.04.2014	Carbomers 35000 / 50000	13194503	1
Caelo	Carbomers 35000 / 50000	14057902	2
Sanacorp	Carbomers 35000 / 50000	1311027-01	1
Caelo	Carbomers 35000 / 50000	14057903	2

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Supplier	Substance	Batch	Spectra
Euro OTC	Carbomers 35000 / 50000	1311027-02	7
Caelo	Carbomers 35000 / 50000	14016209	1
Caelo	Carbomers 35000 / 50000	14149904	1
Caelo	Carbomers 35000 / 50000	14149906	3
Ichthyol/Phönix	Carbomers 35000 / 50000	14149905	1
Sanacaorp	Carbomers 35000 / 50000	14149905	1
Euro OTC	Carbomers 35000 / 50000	130800601	1
Caelo	Carbomers 35000 / 50000	1311027-02	1
Euro OTC	Carbomers 35000 / 50000	1410001-01	12
Caelo	Carbomers 35000 / 50000	14149905	1
Sanacorp	Carbomers 35000 / 50000	14149911	1
Caelo	Carbomers 35000 / 50000	14149911	1
Caelo	Carbomers 35000 / 50000	14149910	2
Caelo	Carbomers 35000 / 50000	15015702	1
Caelo	Carbomers 35000 / 50000	15015703	1
Euro OTC	Carbomers 35000 / 50000	141000-01	1
Euro OTC	Carbomers 35000 / 50000	141000101	1
Caelo	Carbomers 35000 / 50000	15101802	5
Caelo	Carbomers 35000 / 50000	15101801	5
Fischer/Gehe	Carbomers 35000 / 50000	1410001-02	1
Caelo	Carbomers 35000 / 50000	1410001-02	1
Caelo	Carbomers 35000 / 50000	15101809	3
Caelo	Carbomers 35000 / 50000	15101807	2
Caelo	Carbomers 35000 / 50000	15101810	5
Caelo	Carbomers 35000 / 50000	1510801	1
Euro OTC	Carbomers 35000 / 50000	1512010-01	6
EuRho	Carbomers 35000 / 50000	1410001-01	1
Caelo	Carbomers 35000 / 50000	31631293	1
Euro OTC	Carbomers 35000 / 50000	101616773	2
Alliance H.	Carbomers 35000 / 50000	1512010-01	1
Caelo	Carbomers 35000 / 50000	15015709	2
Caelo	Carbomers 35000 / 50000	15439002	6
Euro OTC	Carbomers 35000 / 50000	1512010-02	3
Caelo	Carbomers 35000 / 50000	2215M-01232	1
Euro	Carbomers 35000 / 50000	1410001-01	2
Caelo	Carbomers 35000 / 50000	15257401	1
Euro OTC	Carbomers 35000 / 50000	1604032-01	6
Caelo	Carbomers 35000 / 50000	15439003	9
Euro OTC	Carbomers 35000 / 50000	151210-02	1
Sanacorp	Carbomers 35000 / 50000	1604032-01	1
Euro/Gehe	Carbomers 35000 / 50000	1604032-01	1
Euro OTC	Carbomers 35000 / 50000	1607028-01	6
Caelo	Carbomers 35000 / 50000	16253004	7
Caesar&Loretz,Phönix,06...	Carbomers 35000 / 50000	15439003	1
Sanacorp	Carbomers 35000 / 50000	160702801	1
Euro OTC	Carbomers 35000 / 50000	1610024-01	7
Caelo	Carbomers 35000 / 50000	16253005	4
Caelo	Carbomers 35000 / 50000	16253001	1
Caelo	Carbomers 35000 / 50000	16253007	4
Caelo	Carbomers 35000 / 50000	16237501	1
Euro/Phönix	Carbomers 35000 / 50000	161002401	1
Caelo	Carbomers 35000 / 50000	16253009	7
Nachtestung	Carbomers 35000 / 50000		1
Gehe	Carbomers 35000 / 50000	16237501	1
Caelo	Carbomers 35000 / 50000	16253002	1
Caelo	Carbomers 35000 / 50000	1081702	1
Rezepturlager - Verläng...	Carbomers 35000 / 50000	115/14	1
Caelo	Carbomers 35000 / 50000	16253012	3
Noweda	Carbomers 35000 / 50000	16253012	1
Caelo	Carbomers 35000 / 50000	17146501	1

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Supplier	Substance	Batch	Spectra
Caelo	Carbomers 35000 / 50000	16253014	1
Caelo	Carbomers 35000 / 50000	162530	1
Euro OTC	Carbomers 35000 / 50000	16253014	1
Euro OTC	Carbomers 35000 / 50000	1706015-01	1
Euro OTC	Carbomers 35000 / 50000		1
Caelo	Carbomers 35000 / 50000	17361402	2
Caelo	Carbomers 35000 / 50000	18092401	6
Caelo	Carbomers 35000 / 50000	1706015-01	1
Euro OTC	Carbomers 35000 / 50000	1702012-01	1
Caelo	Carbomers 35000 / 50000	18092402	3
Euro OTC	Carbomers 35000 / 50000	1801044-01	1
Jenne	Carbomers 35000 / 50000	18049301	1
Caelo	Carbomers 35000 / 50000	18092405	1
Euro OTC	Carbomers 35000 / 50000	102026590	1
Caelo	Carbomers 35000 / 50000	9011903	1

- 78 645 spectra from 565 *Apo-Ident* customers from a total of 26 042 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Carbomers 35000 / 50000* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Carbomers 35000 / 50000* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	74 136
Type B	0	380	0	126 512
Type C	0	274	10	78 645

The substance/substance group *Carbomers 35000 / 50000* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.8817 %)	96.4789 % (> 95.4225 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22548	22548	0.00	43.20
22759	22759	0.00	43.46
20978	20978	0.00	41.08
20979	20979	0.00	40.55
21354	22548	3.19	41.94
21561	22548	3.19	43.30
22250	22250	0.00	47.04
22686	22686	0.00	42.77
22852	22852	0.00	42.88

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Carmellose sodium (400 / 450 / 500 / 600 / 1600 ...**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20866-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Carmellose sodium (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s); Carmellosum natricum (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s)

Special notes

When selecting the *Carmellose sodium (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Carmellose sodium (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Carmellose sodiu...	12354404	20866	40	1401185
Caelo	Carmellose sodiu...	13104807	20872	40	1401186
Fagron	Carmellose sodiu...	13D22-N02	20892	40	1401187
Caelo	Carmellose sodiu...	14029211	21382	40	20140127

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Carmellose sodiu...	13299310	21432	40	20131002
Caelo	Carmellose sodiu...	161714	22645	40	20160713*
Caelo	Carmellose sodiu...	16171406	23187	40	AR-17-FG-015964-01
Caelo	Carmellose sodiu...	180486	24039	40	20180228*

Validation samples

A total of 280317 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 *Carmellose sodium* (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s). These samples are listed above in the [calibration samples](#) section.
- 74176 spectra from a total of 1615 batches from further 372 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 *Carmellose sodium* (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s).

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Carmellose sodium (400 / 450...	13299310	21432 [†]	20
Caelo	Carmellose sodium (400 / 450...	17062304	23519	40
Caelo	Carmellose sodium (400 / 450...	172446	23623	40

- 126792 spectra from a total of 2786 batches from further 781 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.

- 47 spectra from 27 *Apo-Ident* customers from 29 batches from the substance/substance group *Carmellose sodium* (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s).

Supplier	Substance	Batch	Spectra
Caelo	Carmellose sodium (400 / 450...	11124211	1
Caelo	Carmellose sodium (400 / 450...	12255708	1
Noweda	Carmellose sodium (400 / 450...	12354401	1
Caelo	Carmellose sodium (400 / 450...	13104802	3
Caelo	Carmellose sodium (400 / 450...	13104810	3
Caelo	Carmellose sodium (400 / 450...	12354408	1
Caelo	Carmellose sodium (400 / 450...	13104813	3
Caelo	Carmellose sodium (400 / 450...	12354416	3
Caelo	Carmellose sodium (400 / 450...	13299302	2
Fagron	Carmellose sodium (400 / 450...	13D22-N02	1
Caelo	Carmellose sodium (400 / 450...	12354414	1
Caelo	Carmellose sodium (400 / 450...	13104807	1
Gutenberg-Apotheke	Carmellose sodium (400 / 450...	4811E-03302	1
Caelo	Carmellose sodium (400 / 450...	28051402	1
Gehe 06.10.14	Carmellose sodium (400 / 450...	13299312	1
Caelo	Carmellose sodium (400 / 450...	13G19-N02	1
Caelo	Carmellose sodium (400 / 450...	14149806	1
Sanacorp	Carmellose sodium (400 / 450...	AKD6	1
Caelo	Carmellose sodium (400 / 450...	14029201	1
Caelo	Carmellose sodium (400 / 450...	15123901	3
Caelo	Carmellose sodium (400 / 450...	14029211	1
Caelo	Carmellose sodium (400 / 450...	15123908	3
Fagron	Carmellose sodium (400 / 450...	15G03-Bo2-312862	1
Caelo	Carmellose sodium (400 / 450...	1315Q-03302	1
Caelo	Carmellose sodium (400 / 450...	16171402	2
Caelo	Carmellose sodium (400 / 450...	17062304	3
Caelo	Carmellose sodium (400 / 450...	17052304	1
Caelo	Carmellose sodium (400 / 450...	17062307	2
Gehe	Carmellose sodium (400 / 450...	17062307	1
Caelo	Carmellose sodium (400 / 450...	25041805	1

- 78 882 spectra from 565 *Apo-Ident* customers from a total of 26 110 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Carmellose sodium* (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s) can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Carmellose sodium* (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s) and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The

following table breaks down the numbers of correct and incorrect results according to 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	74 176
Type B	0	97	3	126 792
Type C	0	46	1	78 882

The substance/substance group *Carmellose sodium* (400 / 450 / 500 / 600 / 1600 / 2000 mPa · s) can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9901 %)	97.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	97.8723 % (> 91.4894 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20866	20866	0.00	56.30
21432	20866	6.57	53.03
20872	20872	0.00	57.41
21382	20872	7.39	61.49
23187	23187	0.00	49.01
22645	22645	0.00	33.99
20892	20892	0.00	52.31
24039	24039	0.00	63.15

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Cellulose, microcrystalline**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20708-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Cellulose, microcrystalline; Cellulosum microcristallinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Cellulose, microcrystalline*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cellulose, micro...	12C23-N06	20708	70	1403080
Euro OTC	Cellulose, micro...	1201004-01	20728	40	20120201
Euro OTC	Cellulose, micro...	1211037-01	21080	30	20121207
Euro OTC	Cellulose, micro...	1507022	21857	40	20150805*
Euro OTC	Cellulose, micro...	1604029	22559	40	20160512*
Fagron	Cellulose, micro...	16B24-B11-323324	22896	40	20160311

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Cellulose, microcrystalline*. These samples are listed above in the [calibration samples](#) section.
- 74 236 spectra from a total of 1617 batches from further 372 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 [†].

- 260 spectra of 7 reference samples from the substance/substance group *Cellulose, microcrystalline*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cellulose, microcrystalline	1211037-01	21085	40
Euro OTC	Cellulose, microcrystalline	1507022	21857 [†]	20
Euro OTC	Cellulose, microcrystalline	1607042	22794	40
Euro OTC	Cellulose, microcrystalline	1604029-01	22815	40
Euro OTC	Cellulose, microcrystalline	1610030	22876	40
Euro OTC	Cellulose, microcrystalline	1712009	23909	40
Euro OTC	Cellulose, microcrystalline	1811011	24346	40

- 126 632 spectra from a total of 2782 batches from further 781 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.

- 41 spectra from 28 *Apo-Ident* customers from 23 batches from the substance/substance group *Cellulose, microcrystalline*.

Supplier	Substance	Batch	Spectra
EuRho	Cellulose, microcrystalline	1201004-02	1
Euro OTC	Cellulose, microcrystalline	1211037-01	2
Koisser	Cellulose, microcrystalline	E0790	1
Euro OTC	Cellulose, microcrystalline	1201004-02	2
Euro OTC	Cellulose, microcrystalline	121103701	1
Fagron	Cellulose, microcrystalline	13A03-N01	1
Euro OTC	Cellulose, microcrystalline	1309001-01	3
Phnoix	Cellulose, microcrystalline	1211037-01	1
Phoenix	Cellulose, microcrystalline	1309001-02	1
Fagron	Cellulose, microcrystalline	9K10-N10	1
Euro OTC	Cellulose, microcrystalline	700204	1
Euro OTC	Cellulose, microcrystalline	1309001-02	3
Euro OTC	Cellulose, microcrystalline	1410002-01	4
Fagron	Cellulose, microcrystalline	2013M-01350	1
Euro OTC	Cellulose, microcrystalline	135010001	1
Fagron	Cellulose, microcrystalline	15C03-B06-305242	1
Euro/Noweda	Cellulose, microcrystalline	1410002-02	1
apo-ident.	Cellulose, microcrystalline	1604029-01	1
Euro OTC	Cellulose, microcrystalline	1604029-01	6
Euro OTC	Cellulose, microcrystalline	150702201	1
Euro OTC	Cellulose, microcrystalline	1607042-01	1
Euro OTC	Cellulose, microcrystalline	150722-01	1
Euro OTC	Cellulose, microcrystalline	1610030-01	1
Fagron	Cellulose, microcrystalline	17A11-B04-331463	1
Euro OTC	Cellulose, microcrystalline	160704201	1
Euro OTC	Cellulose, microcrystalline	1712009-01	1
Euro OTC	Cellulose, microcrystalline	1712009-02	1

- 78 888 spectra from 565 *Apo-Ident* customers from a total of 26 114 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Cellulose, microcrystalline* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cellulose, microcrystalline* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 236
Type B	0	259	1	126 632
Type C	0	40	1	78 888

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9901 %)	99.6154 % (> 98.4615 %)
Type C	100.0000 % (> 99.8817 %)	97.5610 % (> 90.2439 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20708	20708	0.00	70.86
22559	22559	0.00	76.43
20728	20708	3.24	69.36
21080	20708	3.58	67.38
21857	21857	0.00	75.04
22896	21857	2.38	71.63

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Cetostearyl alcohol
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20738-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cetostearyl alcohol; Alcohol cetylicus; Alcohol cetylicus et stearylicus; Alcohol cetylicus et stearylicus emulsificans A; Cetomacrogol emulsifying wax 1000 NI; Cetyl alcohol; Emulsifying cetostearyl alcohol (type A)

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Cetostearyl alcohol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cetomacrogol emu. ...	12H07-N06	20738	30	20120905
Caelo	Cetyl alcohol	13096901	20896	40	1405179
Fagron	Cetostearyl alco. ...	13C13-N13	20968	40	1402265

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cetomacrogol emu...	13C05-B40-289262	21054	40	1408003
Fagron	Emulsifying ceto...	13L17-B05	21279	40	1505070
Caelo	Cetostearyl alco...	14054504	21314	40	20140226
Caelo	Emulsifying ceto...	13233005	21319	30	1506057
Caelo	Cetomacrogol emu...	14055001	21381	40	20140225
Caelo	Cetyl alcohol	13286502	21435	40	20130925
Caelo	Emulsifying ceto...	14322505	21830	40	20141031
Euro OTC	Emulsifying ceto...	1510043	21998	40	20151124*
Euro OTC	Emulsifying ceto...	1504010-01	22264	40	20150423
Caelo	Cetyl alcohol	15323301	22266	40	AR-16-FG-008835-01
Caelo	Emulsifying ceto...	153857	22332	40	20151202*
Caelo	Emulsifying ceto...	153856	22334	40	20160210*
Caelo	Cetomacrogol emu...	15277504	22390	40	20150828
Caelo	Cetomacrogol emu...	160804	22397	40	20160323*
Caelo	Cetyl alcohol	161063	22398	40	20160420*
Caelo	Cetyl alcohol	161063	22403	40	20160420*
Euro OTC	Cetyl alcohol	1508014-01	22611	40	20150821
Fagron	Emulsifying ceto...	16I13-B01-326511	23022	40	20161024
Caelo	Cetostearyl alco...	17049205	23725	40	20170302

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 860 spectra of 22 reference samples from the substance/substance group *Cetostearyl alcohol*. These samples are listed above in the [calibration samples](#) section.
- 73636 spectra from a total of 1602 batches from further 369 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 [†].

- 1070 spectra of 29 reference samples from the substance/substance group *Cetostearyl alcohol*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cetomacrogol emulsifying wax...	12H07-N06	20738 [†]	10

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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	Cetyl alcohol	13286502	21318	40
Caelo	Emulsifying cetostearyl alco...	13233005	21434	60
Caelo	Cetyl alcohol	13286502	21435 [†]	20
Caelo	Cetostearyl alcohol	14054504	21442	60
Caelo	Emulsifying cetostearyl alco...	14322505	21830 [†]	20
Euro OTC	Emulsifying cetostearyl alco...	1510043	21998 [†]	20
Euro OTC	Emulsifying cetostearyl alco...	1504010-01	22264 [†]	20
Caelo	Cetyl alcohol	15323301	22266 [†]	20
Caelo	Emulsifying cetostearyl alco...	153857	22331	60
Caelo	Emulsifying cetostearyl alco...	153857	22332 [†]	20
Caelo	Emulsifying cetostearyl alco...	153856	22333	60
Caelo	Emulsifying cetostearyl alco...	153856	22334 [†]	20
Caelo	Cetomacrogol emulsifying wax...	160804	22395	40
Caelo	Cetomacrogol emulsifying wax...	160804	22396	40
Caelo	Cetyl alcohol	161063	22399	40
Caelo	Cetyl alcohol	161063	22400	40
Caelo	Cetyl alcohol	161063	22401	40
Caelo	Cetyl alcohol	161063	22402	40
Euro OTC	Emulsifying cetostearyl alco...	1604013	22540	40
Euro OTC	Emulsifying cetostearyl alco...	1701031	22999	40
Caelo	Cetyl alcohol	170473	23068	40
Caelo	Cetostearyl alcohol	170492	23097	40
Euro OTC	Emulsifying cetostearyl alco...	1705001	23381	40
Caelo	Emulsifying cetostearyl alco...	171980	23575	40
Euro OTC	Emulsifying cetostearyl alco...	1711001	23737	40
Caelo	Cetostearyl alcohol	172979	23819	40
Caelo	Cetyl alcohol	173155	23973	40
Caelo	Emulsifying cetostearyl alco...	180180	24033	40

- 125 822 spectra from a total of 2767 batches from further 778 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.

- 639 spectra from 239 *Apo-Ident* customers from 234 batches from the substance/substance group *Cetostearyl alcohol*.

Supplier	Substance	Batch	Spectra
Caelo	Emulsifying cetostearyl alco...	25051201	1
Caelo	Emulsifying cetostearyl alco...	18081201	1
Caelo	Emulsifying cetostearyl alco...	11291101	1
Fagron	Emulsifying cetostearyl alco...	11L22-N09	1
Fagron	Emulsifying cetostearyl alco...	12G02-N04	5
Caelo	Emulsifying cetostearyl alco...	12C30-N01	1
Bombastus	Emulsifying cetostearyl alco...	265360	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	Emulsifying cetostearyl alco...	11009204	1
Caelo	Emulsifying cetostearyl alco...	12065709	6
Caesar & Loretz GmbH	Emulsifying cetostearyl alco...	12065703	1
Fagron	Emulsifying cetostearyl alco...	12C30-N01	2
Fagron	Emulsifying cetostearyl alco...	20260712-2	1
Caelo	Emulsifying cetostearyl alco...	12229402	2
Fagron	Emulsifying cetostearyl alco...	8256792	2
Caelo	Emulsifying cetostearyl alco...	11291103	1
Fagron	Emulsifying cetostearyl alco...	12602-N04	1
Caesar/Noweda	Emulsifying cetostearyl alco...	11343405	1
Caelo	Emulsifying cetostearyl alco...	12231402	1
Fagro	Emulsifying cetostearyl alco...	5211Q-01078	1
Sanacorp	Emulsifying cetostearyl alco...	12J29-N04	1
Caelo	Emulsifying cetostearyl alco...	12331402	6
Fagron	Emulsifying cetostearyl alco...	12J29-N04	3
A.H.D.	Emulsifying cetostearyl alco...	12L19-N03	2
Fagron	Emulsifying cetostearyl alco...	12L19-N03	7
Fagron	Emulsifying cetostearyl alco...	12G02N04	1
Bombastus	Emulsifying cetostearyl alco...	278418	1
Anzag	Emulsifying cetostearyl alco...	12G02-N04	1
Caelo	Emulsifying cetostearyl alco...	13144104	2
Caelo	Emulsifying cetostearyl alco...	25/AKD1	1
Caelo	Emulsifying cetostearyl alco...	12331407	3
Caesar/Noweda	Emulsifying cetostearyl alco...	12065707	1
Gehe	Emulsifying cetostearyl alco...	12L19-N03	1
Caelo	Emulsifying cetostearyl alco...	12134203	1
Caelo	Emulsifying cetostearyl alco...	13144107	2
Noweda	Emulsifying cetostearyl alco...	13144104	1
Caelo	Emulsifying cetostearyl alco...	24101305	1
Fagron	Emulsifying cetostearyl alco...	13F07-N05	7
Sanacorp	Emulsifying cetostearyl alco...	13F07-N05	4
Euro OTC	Emulsifying cetostearyl alco...	1305035-01	1
Caelo	Emulsifying cetostearyl alco...	13144105	11
Phoenix 26.11.12	Emulsifying cetostearyl alco...	13144105	1
Caelo	Emulsifying cetostearyl alco...	13233001	1
Caelo	Emulsifying cetostearyl alco...	2011404	1
Caelo	Emulsifying cetostearyl alco...	13233002	2
Caesar/Lorenz	Emulsifying cetostearyl alco...	13233005	1
Caelo	Emulsifying cetostearyl alco...	13233005	11
Phönix	Emulsifying cetostearyl alco...	1323305	1
Caelo	Emulsifying cetostearyl alco...	19032014B	1
PHOENIX am07.04.2014	Emulsifying cetostearyl alco...	13F07-N05	1
Fagron	Emulsifying cetostearyl alco...	13L17-B05-289805	6
Fagron	Emulsifying cetostearyl alco...	13I06-N04	1
Fagron	Emulsifying cetostearyl alco...	9652865	1
Fagron	Emulsifying cetostearyl alco...	13L17-B05-289806	2
Caelo	Emulsifying cetostearyl alco...	Unbekannt	1
Sanacorp	Emulsifying cetostearyl alco...	13I06-N04	1
Fagron	Emulsifying cetostearyl alco...	13L17B05289805	1
Caelo	Emulsifying cetostearyl alco...	13L17-B05-289806	1
Fagron	Emulsifying cetostearyl alco...	13L17-B05	1
Fagron	Emulsifying cetostearyl alco...	3013M-01078	1
Alliance Health 24.07.2...	Emulsifying cetostearyl alco...	13L17-B05-289805	1
Caelo	Emulsifying cetostearyl alco...	23091402	1
Fagron	Emulsifying cetostearyl alco...	13L17-B05-294999	3
Caelo	Emulsifying cetostearyl alco...	14158201	10
Caelo	Emulsifying cetostearyl alco...	13233008	2
Caesar&lorenz,Phoenix	Emulsifying cetostearyl alco...	14158201	1
Caesar & Loretz GmbH	Emulsifying cetostearyl alco...	13233008	1
Caelo	Emulsifying cetostearyl alco...	14158202	1

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Supplier	Substance	Batch	Spectra
Caelo	Emulsifying cetostearyl alco...	5011505	1
Caelo	Emulsifying cetostearyl alco...	14322502	2
Euro OTC	Emulsifying cetostearyl alco...	1404019-01	1
Caelo	Emulsifying cetostearyl alco...	13352102	1
Caelo	Emulsifying cetostearyl alco...	14322505	10
Caelo	Emulsifying cetostearyl alco...	13233006	1
Euro OTC	Emulsifying cetostearyl alco...	1212019-01	1
Caelo	Emulsifying cetostearyl alco...	31032015B	1
Bombastus	Emulsifying cetostearyl alco...	288691	3
alliance health. 05.05...	Emulsifying cetostearyl alco...	14G31-B03-297610	1
Euro OTC	Emulsifying cetostearyl alco...	1404019-02	1
Fagron	Emulsifying cetostearyl alco...	14G31-B03-297610	2
Caelo	Emulsifying cetostearyl alco...	23051503	1
Caelo	Emulsifying cetostearyl alco...	15090701	8
Fagron	Emulsifying cetostearyl alco...	14G31-B03	1
Caelo	Emulsifying cetostearyl alco...		1
Euro OTC	Emulsifying cetostearyl alco...	14G31-B03-297610	1
Caelo	Emulsifying cetostearyl alco...	14322506	1
Fagron	Emulsifying cetostearyl alco...	14G31-B03-305612	3
Caelo	Emulsifying cetostearyl alco...	14G31-B03-305612	3
Sanacorp	Emulsifying cetostearyl alco...	15090701	1
Fagron	Emulsifying cetostearyl alco...	11499002	1
Caelo	Emulsifying cetostearyl alco...	14156201	1
Euro OTC	Emulsifying cetostearyl alco...	1504010-01	2
Fagron	Emulsifying cetostearyl alco...	15C31-B99-307062	3
Caelo	Emulsifying cetostearyl alco...	14322512	1
Fagron	Emulsifying cetostearyl alco...	15D24-B02-308261	5
Phönix	Emulsifying cetostearyl alco...	15C31-B99-307062	2
Euroh/Noweda	Emulsifying cetostearyl alco...	1504010-01	1
Caelo	Emulsifying cetostearyl alco...	15090703	2
Caelo	Emulsifying cetostearyl alco...	15090706	3
Fagron	Emulsifying cetostearyl alco...	15C31-B00-307062	1
Caelo	Emulsifying cetostearyl alco...	15271405	8
Caelo	Emulsifying cetostearyl alco...	15271403	9
Bombastus	Emulsifying cetostearyl alco...	295148	1
Caelo	Emulsifying cetostearyl alco...	15271402	9
Fagron	Emulsifying cetostearyl alco...	15D24-B02-311993	6
Euro/Gehe	Emulsifying cetostearyl alco...	150401-01	1
Caesar&Loretz/Noweda	Emulsifying cetostearyl alco...	15271405	1
Caelo	Emulsifying cetostearyl alco...	15C31-B99-307062	1
Euro OTC	Emulsifying cetostearyl alco...	15271403	1
Euro OTC	Emulsifying cetostearyl alco...	10836573	1
Fagron	Emulsifying cetostearyl alco...	15D24-B02	1
Bombastus	Emulsifying cetostearyl alco...	300132	2
Euro OTC	Emulsifying cetostearyl alco...	150410-01	1
Fagron	Emulsifying cetostearyl alco...	2215I-01078	1
Caelo	Emulsifying cetostearyl alco...	15271407	4
Noweda	Emulsifying cetostearyl alco...	13065576	1
Caelo	Emulsifying cetostearyl alco...	15271410	1
Fagron	Emulsifying cetostearyl alco...	161006CSA	1
Caelo	Emulsifying cetostearyl alco...	15385606	1
Fagron	Emulsifying cetostearyl alco...	16B23-B07-320384	5
Fagron	Emulsifying cetostearyl alco...	16B23-B07-318218	2
Caelo	Emulsifying cetostearyl alco...	13144103	1
Caelo	Emulsifying cetostearyl alco...	15271408	2
Caelo	Emulsifying cetostearyl alco...	15385602	3
Fagron	Emulsifying cetostearyl alco...	16B23-B07	1
ALH	Emulsifying cetostearyl alco...	15271405	1
Fagron	Emulsifying cetostearyl alco...	16B23-B07-323025	3
Caesar & Loretz GmbH	Emulsifying cetostearyl alco...	16119604	3

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Supplier	Substance	Batch	Spectra
Euro OTC	Emulsifying cetostearyl alco...	1510043-01	2
Fagron	Emulsifying cetostearyl alco...	16I13-B01326511	1
Caelo	Emulsifying cetostearyl alco...	16119604	9
Henry Lamotte / Noweda	Emulsifying cetostearyl alco...	300132	1
Caelo	Emulsifying cetostearyl alco...	16119607	2
Bombastus	Emulsifying cetostearyl alco...	303935	1
Caelo	Emulsifying cetostearyl alco...	17056802	1
Caelo	Emulsifying cetostearyl alco...	16238607	5
Euro OTC	Emulsifying cetostearyl alco...	1604013-02	1
Fagron	Emulsifying cetostearyl alco...	16/13-Bo1-327864	1
Fagron	Emulsifying cetostearyl alco...	15789271	1
Caelo	Emulsifying cetostearyl alco...	303935	1
Caeolo	Emulsifying cetostearyl alco...	17056807	1
Caelo	Emulsifying cetostearyl alco...	608/10072017	1
Gehe	Emulsifying cetostearyl alco...	1701031-01	1
Caelo	Emulsifying cetostearyl alco...	15071704	1
Caelo	Emulsifying cetostearyl alco...	9170717	1
Caelo	Emulsifying cetostearyl alco...	17056806	4
Fagron	Emulsifying cetostearyl alco...	16I13-B01	2
Caelo	Emulsifying cetostearyl alco...	17132001	4
Caelo	Emulsifying cetostearyl alco...	15789271	1
Euro OTC	Emulsifying cetostearyl alco...	1701031-01	2
Caesar & Loretz GmbH	Emulsifying cetostearyl alco...	17132001	1
Caelo	Emulsifying cetostearyl alco...	17139201	4
Fagron	Emulsifying cetostearyl alco...	17D28-B06-334609	2
Fagron	Emulsifying cetostearyl alco...	16/13-B01-327355	2
Caelo	Emulsifying cetostearyl alco...	17198003	11
Fagron	Emulsifying cetostearyl alco...	171216CAE/0016830715	1
Caelo	Emulsifying cetostearyl alco...	16238604	1
Caelo	Emulsifying cetostearyl alco...	17261701	1
Fagron	Emulsifying cetostearyl alco...	17D28-B06	1
Caelo	Emulsifying cetostearyl alco...	17261702	2
Euro OTC	Emulsifying cetostearyl alco...	1705001-01	2
Fagron	Emulsifying cetostearyl alco...	17D28-B06-338141	2
Fagron	Emulsifying cetostearyl alco...	17F21-B01-341021	4
Fagron	Emulsifying cetostearyl alco...	18003401	1
Caelo	Emulsifying cetostearyl alco...	17198002	1
Krieger	Emulsifying cetostearyl alco...	1711001-01	1
Bombastus	Emulsifying cetostearyl alco...	18003404	1
Caelo	Emulsifying cetostearyl alco...	18003404	2
Caelo	Emulsifying cetostearyl alco...	29091803	1
Kehr	Emulsifying cetostearyl alco...	18003404	1
Fagron	Emulsifying cetostearyl alco...	18A23-B04-352987	1
Fagron	Cetostearyl alcohol	7886542	1
Fagron	Cetostearyl alcohol	12g02-n04	1
Fagron	Cetostearyl alcohol	11f30-n11	1
Fagron	Cetostearyl alcohol	10F17-N02	1
Caelo	Cetostearyl alcohol	12025301	2
Fagron	Cetostearyl alcohol	11E17-N13	1
Fagron	Cetostearyl alcohol	12G02-N04	7
Fagron	Cetostearyl alcohol	12J17-N05	1
Fagron	Cetostearyl alcohol	12E30-N13	1
Caelo	Cetostearyl alcohol	11162305	1
Euro OTC	Cetostearyl alcohol	20270912-2	1
Sanacorp	Cetostearyl alcohol	575778	1
Caelo	Cetostearyl alcohol	12021304	1
Caesar & Loretz GmbH, 4...	Cetostearyl alcohol	11302101	1
Euro OTC	Cetostearyl alcohol	1204015-01	1
Caelo	Cetostearyl alcohol	12065709	1
Fagron	Cetostearyl alcohol	12J17-N05	2

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Supplier	Substance	Batch	Spectra
Fagron	Cetostearyl alcohol	8256792	2
Noweda	Cetostearyl alcohol	12065709	1
Caesar/Noweda	Cetostearyl alcohol	2911E-01077	2
Caelo	Cetostearyl alcohol	11302101	1
Caelo	Cetostearyl alcohol	14061317	1
Fagron	Cetostearyl alcohol	12/17-N05	1
Fagron	Cetostearyl alcohol	12K22-N03	3
Fagron	Cetostearyl alcohol	12J29-N04	1
Fagron	Cetostearyl alcohol	13C13-N13	1
Fagron	Cetostearyl alcohol	12L19-N03	1
Caelo	Cetostearyl alcohol	13018305	4
Euro OTC	Cetostearyl alcohol	1305035-01	1
Fagron	Cetostearyl alcohol	9652865	1
Caelo	Cetostearyl alcohol	1314405	1
Caelo	Cetostearyl alcohol	13206206	3
Caelo	Cetostearyl alcohol	13144105	1
Euro OTC	Cetostearyl alcohol	1107035-01	1
Sanacorp	Cetostearyl alcohol	13206206	1
Fagron	Cetostearyl alcohol	13L17-B05-289806	3
ahd/lamotte	Cetostearyl alcohol	13210504	1
Fagron	Cetostearyl alcohol	13F07-N05	2
Fagron	Cetostearyl alcohol	13L17-B05	1
Caelo	Cetostearyl alcohol	14054504	4
Caelo	Cetostearyl alcohol	14054508	3
Fagron	Cetostearyl alcohol	13L17-B05-289805	1
Caelo	Cetostearyl alcohol	13233002	1
Euro OTC	Cetostearyl alcohol	1404019-01	1
Fagron	Cetostearyl alcohol	13L17-B05-294999	1
Euro OTC	Cetostearyl alcohol	1404019-02	1
Caelo	Cetostearyl alcohol	14158201	1
Caelo	Cetostearyl alcohol	13018306	1
Caelo	Cetostearyl alcohol	14322506	1
Fagron	Cetostearyl alcohol	3414E-01078	1
Caelo	Cetostearyl alcohol	14322505	1
Caelo	Cetostearyl alcohol	14346201	3
Caelo	Cetostearyl alcohol	14215007	6
Fagron	Cetostearyl alcohol	14346201	1
Fagron	Cetostearyl alcohol	14G31-B03-297611	1
Caelo	Cetostearyl alcohol	15090701	2
Caelo	Cetostearyl alcohol	15271405	2
Euro OTC	Cetostearyl alcohol	15271403	1
Bombastus	Cetostearyl alcohol	295148	1
Caelo	Cetostearyl alcohol	15272702	1
Fagron	Cetostearyl alcohol	15C31-B99-307062	1
Caelo	Cetostearyl alcohol	15272709	6
Fagron	Cetostearyl alcohol	15D24-B02-311993	2
Caelo	Cetostearyl alcohol	14346202	1
Euro OTC	Cetostearyl alcohol	150401001	1
Fagron	Cetostearyl alcohol	16B23-B07-318218	2
Caesar/Noweda	Cetostearyl alcohol	15272705	1
Bombastus	Cetostearyl alcohol	300132	2
Euro OTC	Cetostearyl alcohol	1504010-01	1
Fagron	Cetostearyl alcohol	15D24-B02	1
Fagron	Cetostearyl alcohol	16B23-B07-320384	1
Caelo	Cetostearyl alcohol	16119604	2
Euro OTC	Cetostearyl alcohol	1510043-01	1
Caelo	Cetostearyl alcohol	15272717	4
Gehe	Cetostearyl alcohol	15272717	1
Gehe	Cetostearyl alcohol	15272713	1
Caelo	Cetostearyl alcohol	8041708	1

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Supplier	Substance	Batch	Spectra
Caelo	Cetostearyl alcohol	160914	1
Euro OTC	Cetostearyl alcohol	1604013-02	2
Ebert-Jacobi	Cetostearyl alcohol	16230603	1
Caelo	Cetostearyl alcohol	16238607	1
Caesar & Loretz GmbH	Cetostearyl alcohol	17056806	1
Caelo	Cetostearyl alcohol	17139201	1
Caelo	Cetostearyl alcohol	16230603	1
Caelo	Cetostearyl alcohol	16048812	1
Caelo	Cetostearyl alcohol	171215CSA/15272717	1
Caelo	Cetostearyl alcohol	13-B01-327355	1
Caelo	Cetostearyl alcohol	16238604	1
Euro OTC	Cetostearyl alcohol	17050001-01	1
Fagron	Cetostearyl alcohol	17F21-B01	1
Caelo	Cetostearyl alcohol	17198003	1
Euro OTC	Cetostearyl alcohol	1705001-01	1
Caelo	Cetostearyl alcohol	17049209	2
Caelo	Cetostearyl alcohol	18003404	1
Caelo	Cetostearyl alcohol	18A23-B04	1
Caelo	Cetomacrogol emulsifying wax...		1
AHD	Cetomacrogol emulsifying wax...	8073743	1
Caelo	Cetomacrogol emulsifying wax...	14055002	1
Caelo	Cetomacrogol emulsifying wax...	15113703	1
Caelo	Cetomacrogol emulsifying wax...	15277505	1
Caelo	Cetomacrogol emulsifying wax...	15277501	1
Caelo	Cetomacrogol emulsifying wax...	16080407	1
Caelo	Cetomacrogol emulsifying wax...	16348101	1
Caelo	Cetomacrogol emulsifying wax...	16080403	1
EuRho Anzag ek:3,47EUR	Cetyl alcohol	110505501	1
Fagron	Cetyl alcohol	12A-02N12	1
Finze	Cetyl alcohol	10321703	1
Caelo	Cetyl alcohol	12018605	2
Caelo	Cetyl alcohol	11320702	2
Caelo	Cetyl alcohol	11153405	1
Caelo	Cetyl alcohol	20250112-1	1
Caelo	Cetyl alcohol	12271103	5
Euro OTC	Cetyl alcohol	1206020-01	1
Caelo	Cetyl alcohol	12338604	6
EuRho	Cetyl alcohol	1206020-01	1
Euro OTC	Cetyl alcohol	1105055-01	1
Euro OTC	Cetyl alcohol	1211002-01	2
Caelo	Cetyl alcohol	1212E-01076	1
Caelo	Cetyl alcohol	13096901	5
Phönix	Cetyl alcohol	13096901	1
Caelo	Cetyl alcohol	1112013B	1
Sanacorpaelo /Sanacorp	Cetyl alcohol	1AKS11	1
Caelo	Cetyl alcohol	13096904	2
Caelo	Cetyl alcohol	13210504	9
Phonix	Cetyl alcohol	13210504	1
Caelo	Cetyl alcohol	13286502	5
Caelo	Cetyl alcohol	14262204	5
Caelo	Cetyl alcohol	14349101	13
Caelo	Cetyl alcohol	15323301	5
Caelo	Cetyl alcohol	15323311	8
Euro OTC	Cetyl alcohol	150818C	1
Caelo	Cetyl alcohol	1523316	1
Caelo	Cetyl alcohol	15323316	3
Fagron	Cetyl alcohol	15D24-B02-311993	1
Caelo	Cetyl alcohol	16106307	3
Caelo	Cetyl alcohol	16335802	6
Gatt-Koller	Cetyl alcohol	1690/06162416	1

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Supplier	Substance	Batch	Spectra
Caelo	Cetyl alcohol	16335807	6
Caelo	Cetyl alcohol	28101701	1
Caelo	Cetyl alcohol	17047307	1
Caelo	Cetyl alcohol	17234902	1
Kehr	Cetyl alcohol	17047303	1
AHD	Cetyl alcohol	17321603	1
Caelo	Cetyl alcohol	17321603	2
Caelo	Cetyl alcohol	7071807	1
Caelo	Cetyl alcohol	17321612	2
Caelo	Cetyl alcohol	18153102	1
Fagron	Cetyl alcohol	18A23-B04-349155	1

- 78 290 spectra from 565 *Apo-Ident* customers from a total of 25 905 batches from a further 690 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Cetostearyl 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 *Cetostearyl 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	860	0	73 636
Type B	0	1067	3	125 822
Type C	0	625	14	78 290

The substance/substance group *Cetostearyl 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 % (> 99.9887 %)	100.0000 % (> 99.3023 %)
Type B	100.0000 % (> 99.9901 %)	99.7196 % (> 99.4393 %)
Type C	100.0000 % (> 99.8817 %)	97.8091 % (> 97.3396 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22266	22266	0.00	41.65
21381	22397	5.10	48.27
22398	22398	0.00	41.74
22397	22397	0.00	35.66
22403	22403	0.00	43.10
20738	21054	3.96	47.85
22611	22398	22.61	40.74
21054	21054	0.00	40.72
20968	20968	0.00	43.49
21279	21279	0.00	46.61
21314	21998	9.67	43.13
21319	21319	0.00	48.63
23725	20968	8.71	43.18
21830	21998	1.64	48.01
21998	21998	0.00	47.71
22264	22334	1.25	46.07
22332	22332	0.00	45.33
22334	22334	0.00	46.21
23022	22334	2.24	46.86
20896	20896	0.00	42.61
21435	20896	17.41	41.77
22390	21054	5.65	50.91

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Chloral hydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20322-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Chloral hydrate; Chlorali hydras

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Chloral hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Chloral hydrate	13F06-N07	21231	40	20130626
Caelo	Chloral hydrate	13213311	21309	40	20130712
Caelo	Chloral hydrate	15448318	22963	40	1704462
Caelo	Chloral hydrate	16355802	23094	40	20170112

Validation samples

A total of 280 317 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 *Chloral hydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Chloral hydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Chloral hydrate	154483	23355	40
Fagron	Chloral hydrate	17E05-B05-335580	23572	40
Caelo	Chloral hydrate	172506	23646	40
Caelo	Chloral hydrate	172477	23678	40
Caelo	Chloral hydrate	172477	23815	40

- 126 692 spectra from a total of 2785 batches from further 781 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.

- 229 spectra from 112 *Apo-Ident* customers from 86 batches from the substance/substance group *Chloral hydrate*.

Supplier	Substance	Batch	Spectra
Fagron	Chloral hydrate	12C26-M05	1

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Supplier	Substance	Batch	Spectra
Fagron	Chloral hydrate	12H06-N08	6
Fagron	Chloral hydrate	12C26-M04	1
Caelo	Chloral hydrate	12017512	1
Fagron	Chloral hydrate	11D13-N07	1
Caelo	Chloral hydrate	12017518	1
Caelo	Chloral hydrate	12017503	1
Fagron	Chloral hydrate	11J05-N01	1
Fagron	Chloral hydrate	12H06N08	3
Sanacorp	Chloral hydrate	12H06-N08	3
Phönix Gotha	Chloral hydrate	13F06-N07	2
Fagron	Chloral hydrate	12H06-N080101/1612	1
Caelo	Chloral hydrate	14101307	1
Fagron	Chloral hydrate	13F06-N070631/786	1
Caelo	Chloral hydrate	13002425	2
Caelo	Chloral hydrate	13d22-n11	1
Caelo	Chloral hydrate	25021401	1
Fagron	Chloral hydrate	12H06-N080160/161	1
Ichthyol GmBH	Chloral hydrate	13002425	2
Phönix Gotha	Chloral hydrate	14038302	1
Caelo	Chloral hydrate	13213311	1
Caelo	Chloral hydrate	14038301	2
Caelo	Chloral hydrate	14038311	4
Caelo	Chloral hydrate	14038306	1
Fagron	Chloral hydrate	12H06N8	1
Caelo	Chloral hydrate	1403815	1
Fagron	Chloral hydrate	13F06-N07	2
Caelo	Chloral hydrate	14218701	1
Caelo	Chloral hydrate	14218704	3
Fagron	Chloral hydrate	13D22-N11	1
Caelo	Chloral hydrate	14218705	3
Fagron	Chloral hydrate	13K05-B13	1
Caelo	Chloral hydrate	14218709	5
Fagron	Chloral hydrate	14218710	1
Caelo	Chloral hydrate	3121403	1
Caelo	Chloral hydrate	17121402	1
Sanacorp	Chloral hydrate	14218705	1
Caelo	Chloral hydrate	14218710	1
Caelo	Chloral hydrate	14218714	4
Caelo	Chloral hydrate	14218712	1
Noweda29.04.2015	Chloral hydrate	15083701	2
Fagron	Chloral hydrate	14218712	1
Caelo	Chloral hydrate	14218720	1
Caelo	Chloral hydrate	14218719	4
Caelo	Chloral hydrate	14218713	1
Caelo	Chloral hydrate	15083703	7
Caelo	Chloral hydrate	15083704	1
Caelo	Chloral hydrate	15083701	1
Caelo	Chloral hydrate	15166503	4
Caelo	Chloral hydrate	15083705	1
Caelo	Chloral hydrate	15166501	2
Caelo	Chloral hydrate	15166505	5
Fagron	Chloral hydrate	15166505	1
Caelo	Chloral hydrate	15166502	2
Caelo	Chloral hydrate	15448303	3
Caelo	Chloral hydrate	15166506	6
Fagron	Chloral hydrate	160609/1	1
Caelo	Chloral hydrate	15163901	1
Caelo	Chloral hydrate	15166508	4
Caelo	Chloral hydrate	15166507	5
Caelo	Chloral hydrate	15448306	6

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Supplier	Substance	Batch	Spectra
Caelo	Chloral hydrate	15166513	1
Caelo	Chloral hydrate	160906C	1
Ebert KKH 10.10.16	Chloral hydrate	15448308	1
Caelo	Chloral hydrate	15448304	2
Caelo	Chloral hydrate	15448312	8
Caelo	Chloral hydrate	15448307	2
Caelo	Chloral hydrate	16248703	1
GEHE	Chloral hydrate	15448312	1
Caelo	Chloral hydrate	15448313	6
Caelo	Chloral hydrate	15448315	4
Caesar	Chloral hydrate	15166501	1
Caelo	Chloral hydrate	15448310	1
Caelo	Chloral hydrate	15448318	7
Caelo	Chloral hydrate	15448314	4
Caelo	Chloral hydrate	6051703	1
Caelo	Chloral hydrate	15448322	2
Caelo	Chloral hydrate	15448321	4
Caelo	Chloral hydrate	16355803	1
Caelo	Chloral hydrate	15448320	4
Caelo	Chloral hydrate	15448324	5
Caelo	Chloral hydrate	15448326	4
Gehe	Chloral hydrate	15448326	1
Caelo	Chloral hydrate	17250601	3
Caelo	Chloral hydrate	17247702	4
Caelo	Chloral hydrate	17520601	1
Caelo	Chloral hydrate	17247704	5
Caelo/ Alliance	Chloral hydrate	17247702	1
Caelo	Chloral hydrate	17550601	1
Sanacorp	Chloral hydrate	17346301	1
Caelo	Chloral hydrate	15448325	1
Caelo	Chloral hydrate	17346301	6
Caelo	Chloral hydrate	17346302	3
Caelo	Chloral hydrate	17346303	3
Caelo	Chloral hydrate	30081807	1
Caelo	Chloral hydrate	17346306	5
Fagron	Chloral hydrate	17346301	1
Sanacorp	Chloral hydrate	17346306	1
Caelo	Chloral hydrate	17346307	1
Caelo	Chloral hydrate	17346311	1
Kehr	Chloral hydrate	17346302	1

- 78 700 spectra from 565 *Apo-Ident* customers from a total of 26 051 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Chloral hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chloral hydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	200	0	126 692
Type C	0	228	1	78 700

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8817 %)	99.5633 % (> 98.2533 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21231	22963	6.33	46.64
21309	22963	5.82	46.70
22963	22963	0.00	47.47
23094	22963	3.96	46.64

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Chloramphenicol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20097-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Chloramphenicol; Chloramphenicolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Chloramphenicol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Chloramphenicol	11F20-N05	20777	120	1412249
Caelo	Chloramphenicol	11370716	20787	40	20120202
Caelo	Chloramphenicol	12248507	20807	40	20120831
Euro OTC	Chloramphenicol	1209019-02	20813	80	20130408
Fagron	Chloramphenicol	13A11-N02	20822	40	20130125

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Chloramphenicol	13080924	21701	40	1509287
Euro OTC	Chloramphenicol	1407043-01	21752	40	20140903
Fagron	Chloramphenicol	14E01-B02-308559	21910	40	20140513
Caelo	Chloramphenicol	14346908	21988	40	20150115
Euro OTC	Chloramphenicol	1602002	22367	30	20160309*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 510 spectra of 10 reference samples from the substance/substance group *Chloramphenicol*. These samples are listed above in the [calibration samples](#) section.
- 73 986 spectra from a total of 1613 batches from further 372 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 [†].

- 375 spectra of 11 reference samples from the substance/substance group *Chloramphenicol*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Chloramphenicol	1209019-02	20815	80
Caelo	Chloramphenicol	13080924	21701 [†]	20
Euro OTC	Chloramphenicol	1407043-01	21752 [†]	20
Fagron	Chloramphenicol	14E01-B02-308559	21910 [†]	20
Caelo	Chloramphenicol	14346908	21988 [†]	20
Euro OTC	Chloramphenicol	1602002	22367 [†]	15
Caelo	Chloramphenicol	15358906	22961	40
Fagron	Chloramphenicol	16I12-B07-327124	22962	40
Caelo	Chloramphenicol	162786	23353	40
Euro OTC	Chloramphenicol	1704021	23392	40
Caelo	Chloramphenicol	180178	24049	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*.

- 126 517 spectra from a total of 2778 batches from further 781 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.

- 962 spectra from 344 *Apo-Ident* customers from 209 batches from the substance/substance group *Chloramphenicol*.

Supplier	Substance	Batch	Spectra
Fagron	Chloramphenicol	11/14-N03	2
Euro OTC	Chloramphenicol	1107002-01	2
Caelo	Chloramphenicol	10341717	1
Caelo	Chloramphenicol	11370702	3
Gehe	Chloramphenicol	1107002-02	1
Phönix	Chloramphenicol	10341716	1
Euro OTC	Chloramphenicol	110700202	1
Euro OTC	Chloramphenicol	1107002-02	1
Fagron	Chloramphenicol	12B13-N06	6
Euro OTC	Chloramphenicol	1203012-01	6
Caelo	Chloramphenicol	12072606	1
Caelo	Chloramphenicol	11370705	3
Caelo	Chloramphenicol	11370703	2
Euro OTC	Chloramphenicol		4
Caelo	Chloramphenicol	10341703	1
Anzag ek:2.98EUR 25.08.12	Chloramphenicol	11370711	1
Caelo	Chloramphenicol	11370711	10
Euro OTC	Chloramphenicol	1509211259	1
Caesar & Loretz GmbH	Chloramphenicol	11370711	1
Caelo	Chloramphenicol	11370706	3
Euro OTC	Chloramphenicol	1012013-01	2
Caelo	Chloramphenicol	1137070	1
Sanacorp	Chloramphenicol	11370711	1
Caelo	Chloramphenicol	11370707	2
Caelo	Chloramphenicol	12G02-N01	2
Fagron	Chloramphenicol	11J14-N03	1
Euro OTC	Chloramphenicol	1203012-12	1
Euro OTC	Chloramphenicol	1203012-02	10
Fagron	Chloramphenicol	12G02-N01	9
Euro OTC	Chloramphenicol	2121211203012-0	1
Fragon	Chloramphenicol	12G02-N01	1
Euro OCT	Chloramphenicol	1203012-02	1
Caelo	Chloramphenicol	4712Q-01259	1
Noweda	Chloramphenicol	11370712	1
Caelo	Chloramphenicol	11370713	3
Caelo	Chloramphenicol	11370712	4
Caelo	Chloramphenicol	10341711	2
Fagron	Chloramphenicol	12L11-N06	9
Caelo	Chloramphenicol	10341707	1
Caelo	Chloramphenicol	12g02n01	1
Caelo	Chloramphenicol	12248501	12
Gehe	Chloramphenicol	1203012-01	1

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Supplier	Substance	Batch	Spectra
Caelo	Chloramphenicol	3125204	1
Euro OTC	Chloramphenicol	1209019-01	5
Caelo	Chloramphenicol	11370717	2
Caelo	Chloramphenicol	11370714	2
vdI	Chloramphenicol	12248501	1
Anzag 03.04.13 ek: 3,18EUR	Chloramphenicol	12248501	1
Caelo	Chloramphenicol	11370715	1
EUro/AHD	Chloramphenicol	1209019-01	1
Caelo	Chloramphenicol	1137714	1
Noweda	Chloramphenicol	1137014	1
Caelo	Chloramphenicol	11370716	4
Euro OTC	Chloramphenicol	1209019-02	11
Caelo	Chloramphenicol	12248506	8
Gehe	Chloramphenicol	1209019-02	1
Euro OTC	Chloramphenicol	120901902	2
Fagron	Chloramphenicol	13A11-N02	6
Alliance Health	Chloramphenicol	1209019-02	1
Caelo	Chloramphenicol	12248507	9
Phönix	Chloramphenicol	13A11-N02	3
Euro OTC	Chloramphenicol	1209010-02	3
Caelo	Chloramphenicol	12248505	2
Fagron	Chloramphenicol	13A11N02	1
Fagron	Chloramphenicol	12F01-N23	1
Caelo	Chloramphenicol	DY00911233	1
Northeast Gen	Chloramphenicol	DY122127	1
Caelo	Chloramphenicol	12248509	12
Euro OTC	Chloramphenicol	1302024-01	11
EUro/AHD	Chloramphenicol	1209019-02	1
Caelo	Chloramphenicol	310311	1
AHD	Chloramphenicol	12248507	1
Caelo	Chloramphenicol	1302024-01	1
Euro OTC	Chloramphenicol	1302024-02	6
Sanacorp	Chloramphenicol	41/AKD23	1
Caelo	Chloramphenicol	1302024-02	2
Fagron	Chloramphenicol	12A11-N02	1
Fagron	Chloramphenicol	DY00911233	3
Fagron	Chloramphenicol	13A31-B02-286708	4
Noweda	Chloramphenicol	12248509	1
Caelo	Chloramphenicol	13A31-B02	1
AHD	Chloramphenicol	12248509	1
Caelo	Chloramphenicol	1137004	1
EuRho/Phönix	Chloramphenicol	123012-01	1
Caelo	Chloramphenicol	13080902	1
Caelo	Chloramphenicol	12248524	7
Anzag	Chloramphenicol	1302024-01	1
Fagron	Chloramphenicol	13A31-B02	8
Caelo	Chloramphenicol	12248520	7
Euro OTC	Chloramphenicol	1308017-01	8
Euro OTC	Chloramphenicol	314Q1259	1
Caelo	Chloramphenicol	28011401	1
Caelo	Chloramphenicol	20102012J1	1
Phönix	Chloramphenicol	10341710	1
Sanacorp	Chloramphenicol	120901902	1
Sanacorp	Chloramphenicol	12248501	1
Caelo	Chloramphenicol	11031402	1
Fagron	Chloramphenicol	1202500003	1
Caelo	Chloramphenicol	12248525	6
VDL	Chloramphenicol	1308017-01	1
Caelo	Chloramphenicol	13080903	8
Caelo	Chloramphenicol	1203012-02	1

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Supplier	Substance	Batch	Spectra
EuRho/Phönix	Chloramphenicol	1308017-01	1
PHOENIX 25.04.2014	Chloramphenicol	1308017-02	2
Caelo	Chloramphenicol	13080904	5
Sanacorp	Chloramphenicol	41/AKD24	1
Gutenberg-Apotheke	Chloramphenicol	13A31-B02-286710	1
Euro OTC	Chloramphenicol	1308017-02	8
Phoenix	Chloramphenicol	13080903	1
Caelo	Chloramphenicol	13080303	1
Fagron	Chloramphenicol	13A31-B02-286709	2
AHD	Chloramphenicol	13080904	1
Gatt-Koller / Phoenix	Chloramphenicol	5615/12115211	1
Euro OTC	Chloramphenicol	130801701	1
Caelo	Chloramphenicol	1308017-01	1
Fagron	Chloramphenicol	13A31-B02286708	1
Anzag	Chloramphenicol	1308017-02	1
Nanjing Baijingyu Pharm...	Chloramphenicol	13080908	2
Caelo	Chloramphenicol	13A31-B02-286709	1
Euro/ Sanacorp	Chloramphenicol	1308017-02	1
Caelo	Chloramphenicol	13080907	13
Phönix Gotha	Chloramphenicol	13080907	1
Euro OTC	Chloramphenicol	DY130525	1
Caelo	Chloramphenicol	DY130525	1
Fagron	Chloramphenicol	13A31-B02-290300	3
Bombastus	Chloramphenicol	1308017-01	1
Caelo	Chloramphenicol	13080915	1
ANZAG	Chloramphenicol	1308017-02	1
Caelo	Chloramphenicol	140704301	1
Euro OTC	Chloramphenicol	1407043-01	19
Fagron	Chloramphenicol	13A31-B02-290263	1
Caelo	Chloramphenicol	13080923	11
Phönix	Chloramphenicol	13A1-802	3
Fagron	Chloramphenicol	2111I-01259	1
Caelo	Chloramphenicol	13080917	4
Caelo	Chloramphenicol	13080918	2
noweda	Chloramphenicol	13080908	1
Gehe	Chloramphenicol	1308017-02	1
Phönix	Chloramphenicol	13080921	1
Euro OTC	Chloramphenicol	140704301	4
Caelo	Chloramphenicol	13080921	2
Caelo	Chloramphenicol	4412Q-01259	1
Caelo	Chloramphenicol	13080924	14
VDL	Chloramphenicol	140743-01	1
Sanacorp	Chloramphenicol	140704301	1
Caelo	Chloramphenicol	13080908	3
Fagron	Chloramphenicol	DY00912129	1
Fagron	Chloramphenicol	14E01-B02	4
Euro OTC	Chloramphenicol	T02-55/1407043-01	1
Caelo	Chloramphenicol	93323801	1
Northeast General	Chloramphenicol	1407043-01	1
Euro OTC	Chloramphenicol	1407043	1
Alliance 15.04.2015 Ek ...	Chloramphenicol	1407043-01	1
Caelo	Chloramphenicol	14346901	2
Caelo	Chloramphenicol	14346906	3
Fagron	Chloramphenicol	14E01-B02-296623	1
Caelo	Chloramphenicol	14346904	4
Euro OTC	Chloramphenicol	1502036-01	26
Caelo	Chloramphenicol	14E01-B02-296623	1
Fagron	Chloramphenicol	14E01-B02-306146	5
Caelo	Chloramphenicol	13080925	11
Fagron	Chloramphenicol	14e01-b02-296624	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Chloramphenicol	150203601	5
Euro OTG	Chloramphenicol	1502036-01	1
Fagron	Chloramphenicol	14E01B02296624	2
Caelo	Chloramphenicol	14346907	8
Fagron	Chloramphenicol	14E01-B02-296625	1
Fagron	Chloramphenicol	14E01-B02-296624	3
EuRho / 20	Chloramphenicol	1502036-01	1
Euro/Alliance Healthcare	Chloramphenicol	1502036-01	1
AHDE 20.08.15	Chloramphenicol	DY00912128	1
Fagron	Chloramphenicol	1502036-01	1
Fagron	Chloramphenicol		1
Caelo	Chloramphenicol	1502036-01	2
Fagron	Chloramphenicol	14E01-B02-308559	5
EurPS	Chloramphenicol	1502036-01	2
Euro OTC	Chloramphenicol	DY00912128	2
Euro/Gehe27.10.15	Chloramphenicol	1502036-01	1
Caelo	Chloramphenicol	1407043-01	1
Caelo	Chloramphenicol	14346903	1
Euro OTC	Chloramphenicol	1502036-02	13
Sanacorp	Chloramphenicol	1502036-01	1
Caelo	Chloramphenicol	14346908	7
Noweda	Chloramphenicol	14346901	2
Caelo	Chloramphenicol	14346912	3
Noweda	Chloramphenicol	14346910	1
AHD	Chloramphenicol	14346912	1
Caelo	Chloramphenicol	14346910	10
Caelo	Chloramphenicol	1434608	1
Euro OTC	Chloramphenicol	150203602	1
Euro OTC	Chloramphenicol	1502036022016030911	1
Caelo	Chloramphenicol	1436908	1
Caelo	Chloramphenicol	14346913	8
Northeast General/Noweda	Chloramphenicol	1502036-02	1
Caelo	Chloramphenicol	14E01B02296624	1
Caelo	Chloramphenicol	14346911	17
Caelo	Chloramphenicol	1502036-02	1
Caelo	Chloramphenicol	14346917	6
EuRho	Chloramphenicol	216A-01259	1
Euro OTC	Chloramphenicol	1502036-03	16
Caelo	Chloramphenicol	130416-1	1
Caelo	Chloramphenicol	130416-2	1
Euro OTC	Chloramphenicol	150203603	1
Caelo	Chloramphenicol	14246917	1
Euro OTC	Chloramphenicol	1602002-01	31
Caelo	Chloramphenicol	14346918	16
Caelo	Chloramphenicol	3081602	1
Caelo	Chloramphenicol	1502036-03	2
Caelo	Chloramphenicol	1602002-01	4
Caolo- Noweda	Chloramphenicol	14346908	1
Caelo	Chloramphenicol	14346922	1
Euro OTC	Chloramphenicol	1502036	1
Caelo	Chloramphenicol	14346914	3
Anzag	Chloramphenicol	14346924	2
Caelo	Chloramphenicol	150528C	1
Caelo	Chloramphenicol	15358907	2
Caelo	Chloramphenicol	14346924	5
Caelo	Chloramphenicol	150203603	1
Euro OTC	Chloramphenicol	1602002-02	18
Fagron	Chloramphenicol	15G14-B04-322516	2
Euro OTC	Chloramphenicol	1602002-07	1
Caelo	Chloramphenicol	2181116	1

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Supplier	Substance	Batch	Spectra
Caelo	Chloramphenicol	15358905	11
Caelo	Chloramphenicol	15358903	3
Phoe	Chloramphenicol	15358905	1
Fagron	Chloramphenicol	16/12-B07	1
Caelo	Chloramphenicol	1602002-02	2
Fagron	Chloramphenicol	16112-B07-326036	1
Fagron	Chloramphenicol	1602002-01	2
anzag	Chloramphenicol	15358907	1
Caelo	Chloramphenicol	15358909	5
Euro OTC	Chloramphenicol	1602002-03	22
Northeast General / Gehe	Chloramphenicol	1602002-02	1
Caelo	Chloramphenicol	15358906	7
Fischer/ Noweda	Chloramphenicol	1502036-03	1
Caelo	Chloramphenicol	15358908	10
Caelo	Chloramphenicol		1
Euro OTC	Chloramphenicol	DY00914151	1
Phönix	Chloramphenicol	16112-b07-327124	1
Caelo	Chloramphenicol	160200201	1
Euro OTC	Chloramphenicol	15358906	1
Caelo	Chloramphenicol	15358912	6
Euro OTC	Chloramphenicol	1602002-03	1
Euro/Noweda	Chloramphenicol	1602002-02	1
Caelo	Chloramphenicol	16358909	1
Noweda	Chloramphenicol	1602002-02	1
Caelo	Chloramphenicol	1535896	1
Gehe	Chloramphenicol	15358906	1
Gehe	Chloramphenicol	15358909	1
Caelo	Chloramphenicol	15358913	16
Finteler Apotheke	Chloramphenicol	15358913	1
Fagron	Chloramphenicol	1602002-02	1
Cealo	Chloramphenicol	1602002-03	1
Caelo	Chloramphenicol	1602002-03	1
phönix	Chloramphenicol	15358912	1
Northeast General	Chloramphenicol	DY00914151	1
Fagron	Chloramphenicol	1602002-03	1
Sanacorp	Chloramphenicol	15358913	1
GEHE	Chloramphenicol	160200202	1
Euro OTC	Chloramphenicol	1704021-01	22
Caelo	Chloramphenicol	1704021-01	6
Caelo	Chloramphenicol	16/12-Bo7-329313	1
Euro OTC	Chloramphenicol	160200203	1
Caelo	Chloramphenicol	16278601	1
Caelo	Chloramphenicol	153589	1
Caelo	Chloramphenicol	15358914	12
Caelo	Chloramphenicol	16278608	5
Euro OTC	Chloramphenicol	170402101	1
Fagron	Chloramphenicol	16/12-B07-332100	1
GEHE	Chloramphenicol	16278608	1
Euro OTC	Chloramphenicol	1704021	1
Euro OTC	Chloramphenicol	1602002-04	1
Euro OTC	Chloramphenicol	15358914	1
GEHE	Chloramphenicol	15358914	1
Caelo	Chloramphenicol	16278602	1
Kehr	Chloramphenicol	1704021-01	1
Fagron	Chloramphenicol	16112-B07-326037	1
Caelo	Chloramphenicol	16278606	3
Caelo	Chloramphenicol	17A23-B08-337138	1
Gehe - Hedinger	Chloramphenicol	1704021-01	1
Caelo	Chloramphenicol	16278609	6
Fagron	Chloramphenicol	17A23B08337138	1

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Supplier	Substance	Batch	Spectra
EuRho	Chloramphenicol	1704021-01	2
Northeast General	Chloramphenicol	1704021-01	2
Noweda	Chloramphenicol	1704021-01	2
Euro OTC	Chloramphenicol	1704021-015505	1
Bombastus	Chloramphenicol	1704021-01	1
Euro OTC	Chloramphenicol	1704021-02	15
Caelo	Chloramphenicol	16278009	1
Caelo	Chloramphenicol	16278612	6
Caelo	Chloramphenicol	16278609/180420CA	1
Fagron	Chloramphenicol	17A23-B-08-336728	1
Gehe	Chloramphenicol	1704021-02	1
Caelo	Chloramphenicol	17343802	4
Sanacorp/EuRho	Chloramphenicol	1704021-02	1
Sanacorp	Chloramphenicol	16278612	1
Caelo	Chloramphenicol	16278611	1
EuRho/Noweda	Chloramphenicol	1704021-02	1
Caelo	Chloramphenicol	17343803	5
Caelo	Chloramphenicol	18017802	2
Euro OTC	Chloramphenicol	130801702	1
Euro OTC	Chloramphenicol	1704021-03	4
Fagron	Chloramphenicol	17A23-B08-336728	1
Sanacorp	Chloramphenicol	17343803	1
Caelo	Chloramphenicol	18017806	5
phoenix-06.11.18	Chloramphenicol	17343803	1
Euro OTC	Chloramphenicol	170402103	1
Caelo	Chloramphenicol	18017807	1
Caelo	Chloramphenicol	18017809	2
Euro OTC	Chloramphenicol	1704021-04	2
Eurho Phönix	Chloramphenicol	1704021-02	1
Caelo	Chloramphenicol	181017809	1

- 77 967 spectra from 565 *Apo-Ident* customers from a total of 25 930 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	510	0	73 986
Type B	0	375	0	126 517
Type C	0	958	4	77 967

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.8235 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.4000 %)
Type C	100.0000 % (> 99.8817 %)	99.5842 % (> 99.2723 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20777	20777	0.00	48.40
20813	20777	1.96	47.69
20822	20777	1.94	47.85
21701	21701	0.00	48.06
21752	22367	10.08	49.14
21910	22367	2.56	47.59
22367	22367	0.00	48.17
20787	20777	4.61	47.65
20807	20777	2.42	48.35
21988	20777	4.62	47.25

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Chlorhexidine diacetate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20989-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Chlorhexidine diacetate; Chlorhexidini acetat

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Chlorhexidine diacetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Chlorhexidine di...	12142726	20989	40	1402685
Caelo	Chlorhexidine di...	12142727	21041	40	20120711
Fagron	Chlorhexidine di...	14I08-B02-306223	22280	40	20140922
Caelo	Chlorhexidine di...	154389	22456	40	20160309*
Caelo	Chlorhexidine di...	15438914	22900	40	1704392

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Chlorhexidine di...	15J02-B08-322916	22947	40	20151104
Caelo	Chlorhexidine di...	15438913	23041	40	20160309*
Caelo	Chlorhexidine di...	154389	23042	40	20160309*
Caelo	Chlorhexidine di...	154389	23043	40	20160309*
Caelo	Chlorhexidine di...	15438909	23044	40	20160309*
Caelo	Chlorhexidine di...	154389	23048	40	20160309*
Fagron	Chlorhexidine di...	14I08-B02-306223	22280SI	40	20140922

Validation samples

A total of 280317 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 *Chlorhexidine diacetate*. These samples are listed above in the [calibration samples](#) section.
- 74016 spectra from a total of 1615 batches from further 372 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 [†].

- 280 spectra of 8 reference samples from the substance/substance group *Chlorhexidine diacetate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Chlorhexidine diacetate	14I08-B02-306223	22280 [†]	20
Caelo	Chlorhexidine diacetate	154389	22456 [†]	20
Fagron	Chlorhexidine diacetate	15J02-B08-322916	22946	40
Caelo	Chlorhexidine diacetate	15438914	22951	40
Caelo	Chlorhexidine diacetate	152610	23045	40
Caelo	Chlorhexidine diacetate	171858	23640	40
Fagron	Chlorhexidine diacetate	15J02-B08-322916	22947SI	40
Caelo	Chlorhexidine diacetate	15438914	22951SI	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*.

- 126612 spectra from a total of 2783 batches from further 781 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.

- 378 spectra from 223 *Apo-Ident* customers from 88 batches from the substance/substance group *Chlorhexidine diacetate*.

Supplier	Substance	Batch	Spectra
Anzag	Chlorhexidine diacetate	70558377	1
Caelo	Chlorhexidine diacetate	10154429	1
Caelo	Chlorhexidine diacetate	11204405	1
Ceasar & Loretz GmbH	Chlorhexidine diacetate	80104278	1
Phoenix	Chlorhexidine diacetate	11204408	1
Caelo	Chlorhexidine diacetate	11204401	3
Caelo	Chlorhexidine diacetate	123456	1
Caelo	Chlorhexidine diacetate	11204406	2
Caelo	Chlorhexidine diacetate	11204408	2
Caelo	Chlorhexidine diacetate	10154421	1
Anzag	Chlorhexidine diacetate	12177505	1
Fagron	Chlorhexidine diacetate	12E14-N11	1
Caelo	Chlorhexidine diacetate	91139389	1
Caelo	Chlorhexidine diacetate	9113904	2
Caelo	Chlorhexidine diacetate	10154407	1
Fagron	Chlorhexidine diacetate	1-8991-1-01-01	1
Caelo	Chlorhexidine diacetate	9113903	1
Caelo	Chlorhexidine diacetate	12177505	3
phönix	Chlorhexidine diacetate		1
Caelo	Chlorhexidine diacetate	12177502	1
Caelo	Chlorhexidine diacetate	12177510	8
Caelo	Chlorhexidine diacetate	10154424	1
Caelo	Chlorhexidine diacetate	12142702	2
Caelo	Chlorhexidine diacetate	12142705	3
Caelo	Chlorhexidine diacetate	12142704	5
Caelo	Chlorhexidine diacetate	11204407	1
Caesar&lorenz,Anzag	Chlorhexidine diacetate	12142704	1
Euro OTC	Chlorhexidine diacetate	10154430	1
Caelo	Chlorhexidine diacetate	12142709	1
Phönix	Chlorhexidine diacetate	Retest09113916	1
Alliance Healthcare	Chlorhexidine diacetate	12177510	1
Caelo	Chlorhexidine diacetate	12142720	10
Noweda	Chlorhexidine diacetate	12142720	1
Caelo	Chlorhexidine diacetate	12142704ok	1
Phönix	Chlorhexidine diacetate	9113916	2
Caesar & Loretz GmbH, 4...	Chlorhexidine diacetate	12142720	1
Caelo	Chlorhexidine diacetate	12142715	3
Caelo	Chlorhexidine diacetate	12142725	6
Caelo	Chlorhexidine diacetate	12177504	1
Caelo	Chlorhexidine diacetate	1242720	1
Caelo	Chlorhexidine diacetate	12142726	9
Phoenix	Chlorhexidine diacetate	12142726	1
Caelo	Chlorhexidine diacetate	12142727	9
Caelo	Chlorhexidine diacetate	10154417	1

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Supplier	Substance	Batch	Spectra
Caelo	Chlorhexidine diacetate	31032014B	1
Fagron	Chlorhexidine diacetate	A-130037	1
Noweda	Chlorhexidine diacetate	12142727	1
Fagron	Chlorhexidine diacetate	13E03-B06-287926	2
Caelo	Chlorhexidine diacetate	12142734	11
Caelo	Chlorhexidine diacetate	13177001	4
Sanacorp	Chlorhexidine diacetate		1
Sanacorp	Chlorhexidine diacetate	12142734	1
Phoenix	Chlorhexidine diacetate	12142734	1
Cealo	Chlorhexidine diacetate	13177002	2
GEHE	Chlorhexidine diacetate	12142734	1
Caelo	Chlorhexidine diacetate	13177002	10
Caelo	Chlorhexidine diacetate	13177007	19
Caelo	Chlorhexidine diacetate	23012015D	1
Phoenix	Chlorhexidine diacetate	13177002	1
Caelo	Chlorhexidine diacetate	13177008	4
Caelo	Chlorhexidine diacetate	13177021	14
Caelo	Chlorhexidine diacetate	1072015C	1
Fagron	Chlorhexidine diacetate	13177008	1
Caelo	Chlorhexidine diacetate	1317021	1
Caelo	Chlorhexidine diacetate	13177022	1
Sanacorp	Chlorhexidine diacetate	7/AKD6	1
Caelo	Chlorhexidine diacetate	13177024	5
keine Angabe	Chlorhexidine diacetate	11204402	2
Caelo	Chlorhexidine diacetate	15261005	5
Euro OTC	Chlorhexidine diacetate	15261004	1
Caelo	Chlorhexidine diacetate	15261004	1
Caelo	Chlorhexidine diacetate	15261007	12
Medichem S.A. ES/Noweda	Chlorhexidine diacetate	13177007	1
Caelo	Chlorhexidine diacetate	15261003	7
Caelo	Chlorhexidine diacetate	15261009	12
Caelo	Chlorhexidine diacetate	15261012	6
Caelo	Chlorhexidine diacetate	15438903	10
Caelo	Chlorhexidine diacetate	15261014	18
Caelo	Chlorhexidine diacetate	12177503	2
AHL	Chlorhexidine diacetate	15438903	1
Caelo	Chlorhexidine diacetate	160912CH	1
Caelo	Chlorhexidine diacetate	10154430	2
Fagron	Chlorhexidine diacetate	15261009	1
Caelo	Chlorhexidine diacetate	15438909	2
Caelo	Chlorhexidine diacetate	15438902	5
Gehe	Chlorhexidine diacetate	15438909	1
Wepa/Wepa	Chlorhexidine diacetate	15438902	1
Fagron	Chlorhexidine diacetate	13E03-B06	1
Caelo	Chlorhexidine diacetate	15438911	10
Fagron	Chlorhexidine diacetate	15J02-B08	1
Fagron	Chlorhexidine diacetate	15J02-B08-322916	2
Caelo	Chlorhexidine diacetate	15438917	9
Caelo	Chlorhexidine diacetate	1543909	1
Phoenix	Chlorhexidine diacetate	15438917	1
Phönix	Chlorhexidine diacetate	15438917	1
caesar	Chlorhexidine diacetate	15261014	1
Caelo	Chlorhexidine diacetate	15438914	4
Cordes/Noweda	Chlorhexidine diacetate	15438914	1
Noweda	Chlorhexidine diacetate	15438911	1
phönix	Chlorhexidine diacetate	15438911	1
Caelo	Chlorhexidine diacetate	17185807	5
Caelo	Chlorhexidine diacetate	17185803	4
Euro OTC	Chlorhexidine diacetate	1785805	1
Caelo	Chlorhexidine diacetate	17185808	6

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Supplier	Substance	Batch	Spectra
Noweda	Chlorhexidine diacetate	17185805	1
Caelo	Chlorhexidine diacetate	17185804	9
Caelo	Chlorhexidine diacetate	17185802	1
Jenne	Chlorhexidine diacetate	17185808	1
Noweda	Chlorhexidine diacetate	17185808	1
Bomastus / Alliance Hea...	Chlorhexidine diacetate	17185804	1
cealo	Chlorhexidine diacetate	17185804	1
Noweda	Chlorhexidine diacetate	1785803	1
Caelo	Chlorhexidine diacetate	180130CA/17185804	1
Caelo	Chlorhexidine diacetate	17185811	8
Noweda	Chlorhexidine diacetate	17185811	1
Fagron	Chlorhexidine diacetate	17185811	1
Caelo	Chlorhexidine diacetate	17188504	1
Caelo	Chlorhexidine diacetate	17185812	7
Sanacorp	Chlorhexidine diacetate	17185804	1
AHD	Chlorhexidine diacetate	17185812	1
Caelo	Chlorhexidine diacetate	17185810	4
Euro OTC	Chlorhexidine diacetate	17185810	3
Caelo	Chlorhexidine diacetate	17325803	9
Caelo	Chlorhexidine diacetate	19121804	1

- 78 551 spectra from 565 *Apo-Ident* customers from a total of 26 051 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Chlorhexidine diacetate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chlorhexidine diacetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 016
Type B	0	280	0	126 612
Type C	0	362	16	78 551

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.9817 %)	95.7672 % (> 94.9735 %)

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

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

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
23048	23048	0.00	26.09
23042	23042	0.00	26.04
23043	23043	0.00	26.19
22280	23044	3.12	26.32
22947	22456	2.44	25.86
23041	23041	0.00	25.98
23044	23044	0.00	26.02
20989	20989	0.00	25.56
21041	22456	7.88	25.56
22456	22456	0.00	25.87
22900	22900	0.00	32.28

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Chlorocresol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20185-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Chlorocresol; Chlorocresolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Chlorocresol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Chlorocresol	13275106	21512	40	20130828
Caelo	Chlorocresol	13275106	21513	40	20130828
Caelo	Chlorocresol	163378	23357	40	20170124*
Caelo	Chlorocresol	182523	24406	40	20180919*

Validation samples

A total of 280 317 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 *Chlorocresol*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1620 batches from further 372 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 *Chlorocresol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Chlorocresol	1211107	21306	40
Caelo	Chlorocresol	13275106	21512 [†]	20
Caelo	Chlorocresol	13275106	21513 [†]	20
Caelo	Chlorocresol	15114107	23411	40
Caelo	Chlorocresol	181360	24050	40

- 126 732 spectra from a total of 2785 batches from further 781 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*.

- 18 spectra from 13 *Apo-Ident* customers from 11 batches from the substance/substance group *Chlorocresol*.

Supplier	Substance	Batch	Spectra
Caelo	Chlorocresol	10145239	3
Caelo	Chlorocresol	7061304	1
Noweda	Chlorocresol	12111017	1
Caelo	Chlorocresol	12111017	2
Caelo	Chlorocresol	12111013	2
Caesar & Loretz GmbH	Chlorocresol	12111017	1
Caelo	Chlorocresol	13275117	1
Caelo	Chlorocresol	2041513	1
Caelo	Chlorocresol	23415422	1
Caelo	Chlorocresol	15114107	1
Caelo	Chlorocresol	4613M-01260	1
Caelo	Chlorocresol	18027101	2
Caelo	Chlorocresol	20101808	1

- 78 911 spectra from 565 *Apo-Ident* customers from a total of 26 126 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Chlorocresol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chlorocresol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	136	24	126 732
Type C	0	17	1	78 911

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	85.0000 % (> 83.1250 %)
Type C	100.0000 % (> 99.9817 %)	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
23357	23357	0.00	28.87
21512	24406	6.24	46.91
24406	24406	0.00	40.38
21513	24406	9.56	39.67

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Chlortetracycline hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20845-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chlortetracycline hydrochloride; Chlortetracyclini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Chlortetracycline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Chlortetracyclin...	12K30-N07	20845	40	1405318
Fagron	Chlortetracyclin...	12K30-N07	21222	40	20121210
Euro OTC	Chlortetracyclin...	1108051-02	21241	40	20111013
Fagron	Chlortetracyclin...	14J08-B07-307742	21877	40	20141029
Euro OTC	Chlortetracyclin...	1604015	22541	40	20160510*

Validation samples

A total of 280317 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 *Chlortetracycline - hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1619 batches from further 372 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 *Chlortetracycline - hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Chlortetracycline hydrochlor...	14J08-B07-307742	21877 [†]	20
Euro OTC	Chlortetracycline hydrochlor...	1604015-01	22975	40
Fagron	Chlortetracycline hydrochlor...	16B10-B09-329778	23571	30
Euro OTC	Chlortetracycline hydrochlor...	1803037	24092	40

- 126762 spectra from a total of 2785 batches from further 781 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*.

- 159 spectra from 100 *Apo-Ident* customers from 48 batches from the substance/substance group *Chlortetracycline hydrochloride*.

Supplier	Substance	Batch	Spectra
Euro OTC	Chlortetracycline hydrochlor...	1108051-01	6
Euro OTC	Chlortetracycline hydrochlor...	2901009V-03	1
Noweda	Chlortetracycline hydrochlor...	12c16-n01	1
Anzag; 07.09.12 ek:4.01	Chlortetracycline hydrochlor...	12C16-N01	1
Caesar & Loretz GmbH	Chlortetracycline hydrochlor...	12C16-N01	1
Fagron	Chlortetracycline hydrochlor...	12C16-N01	1
Krieger	Chlortetracycline hydrochlor...	12C16-No1	1
Caelo	Chlortetracycline hydrochlor...	1108051-01	3
Sanacorp	Chlortetracycline hydrochlor...	1108051-01	1
Fagron	Chlortetracycline hydrochlor...	12H28-N09	4
Fagron	Chlortetracycline hydrochlor...	12K30-N07	8
Fagron	Chlortetracycline hydrochlor...	12H28N09	1
EUro/AHD	Chlortetracycline hydrochlor...	1108051-02	1
Alliance Healthcare	Chlortetracycline hydrochlor...	12K30-N07	1
Euro OTC	Chlortetracycline hydrochlor...	1108051-02	7
Fagron	Chlortetracycline hydrochlor...	12k30-N07	1
Euro OTC	Chlortetracycline hydrochlor...	5113I01155	1
Fagron	Chlortetracycline hydrochlor...	27121306	1
Euro	Chlortetracycline hydrochlor...	1108051-02	1
Euro OTC	Chlortetracycline hydrochlor...	110805102	1
Phoenix	Chlortetracycline hydrochlor...	110805102	1
Fagron	Chlortetracycline hydrochlor...	FC13030134	1
Fagron	Chlortetracycline hydrochlor...	13/11-N07	2
Fagron	Chlortetracycline hydrochlor...	13111-N07	1
Phönix	Chlortetracycline hydrochlor...	1108051-02	2
Fagron	Chlortetracycline hydrochlor...	13K26-N06	1
Fagron	Chlortetracycline hydrochlor...	FC11051038	1
Caelo	Chlortetracycline hydrochlor...	FC13030134	1
Euro OTC	Chlortetracycline hydrochlor...	4612Q-01155	1
Caelo	Chlortetracycline hydrochlor...	14J08-B07-300249	1
Fagron	Chlortetracycline hydrochlor...	14J08-B07	4
Fagron	Chlortetracycline hydrochlor...	14J08-B07-300250	7
Euro OTC	Chlortetracycline hydrochlor...	1412008-01	5
Caelo	Chlortetracycline hydrochlor...	1412008-01	1
Fiebig	Chlortetracycline hydrochlor...	1412008-01	1
Euro OTC	Chlortetracycline hydrochlor...	1412008-02	15
Nachprüfung 2574	Chlortetracycline hydrochlor...	1108051-01	1
Fagron	Chlortetracycline hydrochlor...	14J08-B07-303352	4
Fagron	Chlortetracycline hydrochlor...	14J08-B07-307100	6
Euro OTC	Chlortetracycline hydrochlor...	141200802	2
Sanacop	Chlortetracycline hydrochlor...	1412008-02	1
Fagron	Chlortetracycline hydrochlor...	14J08B07307100	3
Caelo	Chlortetracycline hydrochlor...	141200802	1
Euro OTC	Chlortetracycline hydrochlor...	1412008-03	5
Fagron	Chlortetracycline hydrochlor...	14J08-B07-303350	1
Fagron	Chlortetracycline hydrochlor...	16B10-B09-318088	4
Caelo	Chlortetracycline hydrochlor...	142008-03	1
Caelo	Chlortetracycline hydrochlor...	14J08-B07-303352	1
Caelo	Chlortetracycline hydrochlor...		1
Euro OTC	Chlortetracycline hydrochlor...	1604015-01	15
Fagron	Chlortetracycline hydrochlor...	FC15100204	2
ALH	Chlortetracycline hydrochlor...	16B10-B09-320304	1
Caelo	Chlortetracycline hydrochlor...	141200803	1
Caelo	Chlortetracycline hydrochlor...	16B10-B09-318088	1
Fagron	Chlortetracycline hydrochlor...	16B10-B09-320304	1
Gehe	Chlortetracycline hydrochlor...	16B10-B09	1
Fagron	Chlortetracycline hydrochlor...	16B10-B09-322715	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Chlortetracycline hydrochlor...	10I29-N04	1
EuRo/Phönix	Chlortetracycline hydrochlor...	160401501	1
Gehe	Chlortetracycline hydrochlor...	16B10-B09-322716	1
Fagron	Chlortetracycline hydrochlor...	16B10-B09-326865	1
Phoenix	Chlortetracycline hydrochlor...	16B10-B09-322716	1
Gehe	Chlortetracycline hydrochlor...	16B10-B09-322715	1
Anzag	Chlortetracycline hydrochlor...	1604015-01	1
GEHE	Chlortetracycline hydrochlor...	1604015-01	1
Fagron	Chlortetracycline hydrochlor...	16B10-B09-336332	3
Fagron	Chlortetracycline hydrochlor...	16B10-B09	1
Caelo	Chlortetracycline hydrochlor...	1604015-01	2
Caelo	Chlortetracycline hydrochlor...	16B10-B09-347439	1
Fagron	Chlortetracycline hydrochlor...	16B10-B09-351565	1
Fagron	Chlortetracycline hydrochlor...	16B10-B09-348359	1

- 78 770 spectra from 565 *Apo-Ident* customers from a total of 26 089 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Chlortetracycline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chlortetracycline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	130	0	126 762
Type C	0	148	11	78 770

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.8817 %)	93.0818 % (> 91.1950 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
22541	22541	0.00	31.11
20845	20845	0.00	28.78
21222	20845	3.01	30.07
21241	20845	6.14	28.33
21877	22541	5.96	34.10

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Cholecalciferol dry concentrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20921-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cholecalciferol dry concentrate; Cholecalciferolum pulveratum

Special notes

When selecting the *Cholecalciferol dry concentrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Cholecalciferol dry concentrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cholecalciferol ...	1210051-01	20921	40	1403341
Euro OTC	Cholecalciferol ...	1502021-01	21914	40	20150309
Euro OTC	Cholecalciferol ...	1508032	21949	40	20150901*
Euro OTC	Cholecalciferol ...	1701053	23007	40	20170208*
Euro OTC	Cholecalciferol ...	1801038	23965	40	20180206*

Validation samples

A total of 280317 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 *Cholecalciferol dry concentrate*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 10 reference samples from the substance/substance group *Cholecalciferol dry concentrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cholecalciferol dry concentr...	1304016-02	21240	40
Euro OTC	Cholecalciferol dry concentr...	1502021-01	21914 [†]	20
Euro OTC	Cholecalciferol dry concentr...	1508032	21949 [†]	20
Euro OTC	Cholecalciferol dry concentr...	1602019	22504	40
Euro OTC	Cholecalciferol dry concentr...	1608002	22749	40
Euro OTC	Cholecalciferol dry concentr...	1707027	23740	40
Euro OTC	Cholecalciferol dry concentr...	1802014	23944	40
Euro OTC	Cholecalciferol dry concentr...	1806003	24158	40
Euro OTC	Cholecalciferol dry concentr...	1812010	24416	40
Euro OTC	Cholecalciferol dry concentr...	1901050	24458	40

- 126532 spectra from a total of 2779 batches from further 781 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.

- 12 spectra from 9 *Apo-Ident* customers from 9 batches from the substance/substance group *Cholecalciferol dry concentrate*.

Supplier	Substance	Batch	Spectra
Euro OTC	Cholecalciferol dry concentr...	1012025-01	1
Euro OTC	Cholecalciferol dry concentr...	1210051-01	1
Euro OTC	Cholecalciferol dry concentr...	L1403012-01	1
Euro OTC	Cholecalciferol dry concentr...	1502021-01	1
Euro OTC	Cholecalciferol dry concentr...	1508032-01	2
Euro OTC	Cholecalciferol dry concentr...	1602019-01	1
Caelo	Cholecalciferol dry concentr...	1602019-01	1
Euro OTC	Cholecalciferol dry concentr...	1707027-01	1
Euro OTC	Cholecalciferol dry concentr...	150803201	1
Euro OTC	Cholecalciferol dry concentr...	1801038-01	2

- 78 917 spectra from 565 *Apo-Ident* customers from a total of 26 128 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Cholecalciferol dry concentrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cholecalciferol dry concentrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	356	4	126 532
Type C	0	11	1	78 917

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	98.8889 % (> 98.0556 %)
Type C	100.0000 % (> 99.8818 %)	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
20921	20921	0.00	42.39
23007	23007	0.00	44.58
23965	23965	0.00	41.81
21914	21949	1.92	22.85
21949	21949	0.00	22.87

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Cholesterol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20446-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Cholesterol; Cholesterolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Cholesterol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cholesterol	13F10-B40	21219	40	20131223
Caelo	Cholesterol	160444	22461	40	20160222*
Fagron	Cholesterol	15J23-B03-325106	22971	20	20151103
Caelo	Cholesterol	16044415	23760	40	1804387
Fagron	Cholesterol	17E17-B05-339074	23937	40	20170620

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 5 reference samples from the substance/substance group *Cholesterol*. These samples are listed above in the [calibration samples](#) section.
- 74 316 spectra from a total of 1618 batches from further 372 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 *Cholesterol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cholesterol	13148703	21310	40
Caelo	Cholesterol	160444	22461 [†]	20
Fagron	Cholesterol	15J23-B03-325106	22971 [†]	20
Fagron	Cholesterol	16G05-B03-331396	23522	40

- 126 772 spectra from a total of 2785 batches from further 781 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*.

- 80 spectra from 48 *Apo-Ident* customers from 54 batches from the substance/substance group *Cholesterol*.

Supplier	Substance	Batch	Spectra
Fagron	Cholesterol	10B15-N07	1
Caelo	Cholesterol	11242103	1
Fagron	Cholesterol	2013U-01270	1
Fagron	Cholesterol	10H24-N06	1
Caelo	Cholesterol	12155605	1
Caelo	Cholesterol	13056903	1
Fagron	Cholesterol	13C25-N12	2
Fagron	Cholesterol	12I13-N02	2
Fagron	Cholesterol	13G10-N11	3
Fagron	Cholesterol	8J28-N10	1
Fagron	Cholesterol	12D02-N10	1
Caelo	Cholesterol	12248403	1
Caelo	Cholesterol	14027201	1
Fagron	Cholesterol	13F10-B40-289016	2
Caelo	Cholesterol	14122501	2
Caelo	Cholesterol	13148704	1
Fagron	Cholesterol	11A17-N07	1
Fagron	Cholesterol	13F10-B40	1
Fagron	Cholesterol	14B27-B05-293548	2
Fagron	Cholesterol	14B27-B05	1
Fagron	Cholesterol	14G04-B02-300830	2
Fagron	Cholesterol	14B27-B05-293550	1
Fagron	Cholesterol	14G04-B02	1
Caelo	Cholesterol	15028303	1
Caelo	Cholesterol	14208602	1
Fagron	Cholesterol	15G31-B05-312378	1
Fagron	Cholesterol	15B09-B02	1
Caelo	Cholesterol	15301803	1
Fagron	Cholesterol	15G31-B05	2
Fagron	Cholesterol	15B09-B02-308259	3
Caelo	Cholesterol	15G31-B05-312376	1
Fagron	Cholesterol	15G31-B05-314182	2
Fagron	Cholesterol	15G31-B05-312377	1
Fagron	Cholesterol		1
Caelo	Cholesterol	15B09-B02-308259	1
Fagron	Cholesterol	15B09	1
Caelo	Cholesterol	15358801	5
Fagron	Cholesterol	15G31-B05-316721	1
Fagron	Cholesterol	15J23-B03-320483	4
Caelo	Cholesterol	15407101	2
Caelo	Cholesterol	15J23-B03	1
Caelo	Cholesterol	15407102	1
Noweda	Cholesterol	15J23-B03-320483	1
Fagron	Cholesterol	15J23-B03-322902	1
Fagron	Cholesterol	15J23B03320483	1
Ebert-Jacobi	Cholesterol	16044408	1
Fagron	Cholesterol	15J23-B03-325106	1
Caelo	Cholesterol	16G05-B03	1
Caelo	Cholesterol	16044408	1
Ensbona /Alliance Healt...	Cholesterol	17E17-B05-339074	3
Fagron	Cholesterol	15J23-B03-328249	1
Caelo	Cholesterol	27212	1
Fagron	Cholesterol	15G31-B05316721	1
Fagron	Cholesterol	17K16-B11-343922	2
Fagron	Cholesterol	16G05-B03-334366	1
Fagron	Cholesterol	17K16-B11-348761	1
Fagron	Cholesterol	17E17-B05-337588	1

- 78 849 spectra from 565 *Apo-Ident* customers from a total of 26 083 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	180	0	74 316
Type B	0	120	0	126 772
Type C	0	77	3	78 849

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	96.2500 % (> 92.5000 %)

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
21219	23760	3.08	35.07
22461	22461	0.00	36.38
22971	23760	3.44	33.79
23760	23760	0.00	35.67
23937	23760	14.02	29.30

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Choline chloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	22639-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Choline chloride; Cholinii chloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Choline chloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Choline chloride	162092	22639	40	20160801*
Caelo	Choline chloride	14273819	22663	40	20141002
Caelo	Choline chloride	16209209	23582	40	20160801

Validation samples

A total of 280 317 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 *Choline chloride*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Choline chloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Choline chloride	14273819	22734	40
Caelo	Choline chloride	172053	23618	40
Caelo	Choline chloride	181082	24264	40

- 126 772 spectra from a total of 2786 batches from further 781 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 *Choline chloride*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded 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 *Choline chloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Choline chloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	120	0	126 772
Type C	0	0	0	78 929

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
22639	22639	0.00	104.36
22663	22639	10.73	104.11
23582	22639	7.28	104.59

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Choline hydrogen tartrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20719-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Choline hydrogen tartrate; Cholinium bitartaricum

Special notes

When selecting the *Choline hydrogen tartrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Choline hydrogen tartrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Choline hydrogen...	1603044	22549	40	20160429*
Euro OTC	Choline hydrogen...	1607020	22689	40	20160808*
Euro OTC	Choline hydrogen...	1603044-01	23010	40	20160429
Euro OTC	Choline hydrogen...	1702005	23130	40	20170307*

Validation samples

A total of 280 317 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 *Choline hydrogen tartrate*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 6 reference samples from the substance/substance group *Choline hydrogen tartrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Choline hydrogen tartrate	L1208016-01	20719	40
Euro OTC	Choline hydrogen tartrate	L1208016-02	21242	40
Euro OTC	Choline hydrogen tartrate	1603044-01	23101	40
Euro OTC	Choline hydrogen tartrate	1707023	23610	40
Euro OTC	Choline hydrogen tartrate	1711022	23903	40
Euro OTC	Choline hydrogen tartrate	1802008	23958	40

- 126 652 spectra from a total of 2783 batches from further 781 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.

- 7 spectra from 3 *Apo-Ident* customers from 5 batches from the substance/substance group *Choline hydrogen tartrate*.

Supplier	Substance	Batch	Spectra
Euro OTC	Choline hydrogen tartrate	1309023-01	2
Euro OTC	Choline hydrogen tartrate	1603044-01	1
Euro OTC	Choline hydrogen tartrate	1607020-01	2
Euro OTC	Choline hydrogen tartrate	1707023-01	1
Euro OTC	Choline hydrogen tartrate	1711022-01	1

- 78 922 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Choline hydrogen tartrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Choline hydrogen tartrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	239	1	126 652
Type C	0	7	0	78 922

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	99.5833 % (> 98.3333 %)
Type C	100.0000 % (> 99.8818 %)	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
22549	22549	0.00	69.31
22689	22689	0.00	69.29
23010	22549	1.78	68.32
23130	23130	0.00	61.83

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ciclopirox olamine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20601-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ciclopirox olamine; Ciclopirox olaminum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ciclopirox olamine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ciclopirox olamine	13A16-N04	21218	40	20130117
Caelo	Ciclopirox olamine	13343209	21298	40	AR-15-FG-016214-01
Caelo	Ciclopirox olamine	14147406	21655	40	AR-15-FG-014857-01
Fagron	Ciclopirox olamine	14F13-B03-302340	21964	40	1608170
Caelo	Ciclopirox olamine	14378809	21991	40	20150227

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ciclopirox olamine	15364408	23011	40	20151201
Fagron	Ciclopirox olamine	16G26-B02-324884	23108	40	20160907
Caelo	Ciclopirox olamine	14147406	21655SI	40	AR-15-FG-014857-01
Fagron	Ciclopirox olamine	14F13-B03-302340	21964SI	40	1608170
Caelo	Ciclopirox olamine	14378809	21991SI	40	20150227
Caelo	Ciclopirox olamine	15364408	23011SI	40	20151201

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 11 reference samples from the substance/substance group *Ciclopirox olamine*. These samples are listed above in the [calibration samples](#) section.
- 74056 spectra from a total of 1616 batches from further 372 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 13 reference samples from the substance/substance group *Ciclopirox olamine*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ciclopirox olamine	12040906	20648	40
Fagron	Ciclopirox olamine	14E21-M04	21594	60
Caelo	Ciclopirox olamine	14147406	21655 [†]	20
Fagron	Ciclopirox olamine	14F13-B03-302340	21964 [†]	20
Caelo	Ciclopirox olamine	14378809	21991 [†]	20
Fagron	Ciclopirox olamine	16G26-B02-324884	22969	40
Caelo	Ciclopirox olamine	182102	24280	40
Fagron	Ciclopirox olamine	14E21-M04	21594SI	60
Caelo	Ciclopirox olamine	14147406	21655SI [†]	20
Fagron	Ciclopirox olamine	14F13-B03-302340	21964SI [†]	20
Caelo	Ciclopirox olamine	14378809	21991SI [†]	20
Fagron	Ciclopirox olamine	16G26-B02-324884	22969SI	40
Fagron	Ciclopirox olamine	16G26-B02-324884	23108SI	40

[†]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*.

- 126 452 spectra from a total of 2782 batches from further 781 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.

- 98 spectra from 48 *Apo-Ident* customers from 49 batches from the substance/substance group *Ciclopirox olamine*.

Supplier	Substance	Batch	Spectra
Caelo	Ciclopirox olamine	12B22-N03	1
Noweda	Ciclopirox olamine	12B22-N03	1
Fagron	Ciclopirox olamine	12G12-N09	2
Fagron	Ciclopirox olamine	10L09-N03	1
Fagron	Ciclopirox olamine	13A16-N04	1
Noweda	Ciclopirox olamine	12040911	1
Caelo	Ciclopirox olamine	12040911	1
Phönix	Ciclopirox olamine	13A16-N04	1
Caelo	Ciclopirox olamine	12040906	1
Cael	Ciclopirox olamine	12040911	2
Fagron	Ciclopirox olamine	11h03-n02	1
Caelo	Ciclopirox olamine	13343	1
Caelo	Ciclopirox olamine	13343208	2
Caelo	Ciclopirox olamine	13343209	3
Caelo	Ciclopirox olamine	14147402	4
Fagron	Ciclopirox olamine	14E21-M05	1
Caelo	Ciclopirox olamine	14147405	1
Caelo	Ciclopirox olamine	14147403	2
Caelo	Ciclopirox olamine	14275802	2
Caelo	Ciclopirox olamine	14275801	2
Caelo	Ciclopirox olamine	15018802	2
Caelo	Ciclopirox olamine	13343203	1
Gehe	Ciclopirox olamine	14E21-M04	1
Caelo	Ciclopirox olamine	15018803	1
Caelo	Ciclopirox olamine	14378801	2
Caelo	Ciclopirox olamine	14378803	1
Caelo	Ciclopirox olamine	14378805	2
Caelo	Ciclopirox olamine	14378806	3
Caelo	Ciclopirox olamine	14378810	4
Caelo	Ciclopirox olamine	14378802	1
Caelo	Ciclopirox olamine	15364402	2
Fagron	Ciclopirox olamine	14F13-B03-302339	1
Caelo	Ciclopirox olamine	15364405	2
Caelo	Ciclopirox olamine	15364404	1
Caelo	Ciclopirox olamine	15364407	3
Caelo	Ciclopirox olamine	15364408	4
Caelo	Ciclopirox olamine	15364409	1
Caelo	Ciclopirox olamine	15364412	4
Caelo	Ciclopirox olamine	13343201	1
Caelo	Ciclopirox olamine	15304407	1
Phoenix	Ciclopirox olamine	15364412	1
Sanacorp	Ciclopirox olamine	17118806	1
Caelo	Ciclopirox olamine	15364416	2
Caelo	Ciclopirox olamine	17118806	7

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Supplier	Substance	Batch	Spectra
Euro OTC	Ciclopirox olamine	17118806	1
Euro OTC	Ciclopirox olamine	1718806	1
Fagron	Ciclopirox olamine	A160013	1
GEHE	Ciclopirox olamine	15364405	1
Caelo	Ciclopirox olamine	17118802	3
Caelo	Ciclopirox olamine	17118801	2
Caelo	Ciclopirox olamine	17118808	2
Caelo	Ciclopirox olamine	17118807	2
Caelo	Ciclopirox olamine	16G26-B02-337355	1
Caelo	Ciclopirox olamine	17118811	1
Caesar & Lorenz GmbH	Ciclopirox olamine	171188007	1
Caelo	Ciclopirox olamine	173074055727	1
Caelo	Ciclopirox olamine	17307405	1

- 78 831 spectra from 565 *Apo-Ident* customers from a total of 26 088 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	440	0	74 056
Type B	0	439	1	126 452
Type C	0	93	5	78 831

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9901 %)	99.7727 % (> 99.0909 %)
Type C	100.0000 % (> 99.8817 %)	94.8980 % (> 91.8367 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21218	21964	5.14	80.02
21964	21964	0.00	77.45
23108	21964	4.70	79.42
23011	21298	3.73	82.00
21655	21655	0.00	87.45
21298	21298	0.00	81.17
21991	21298	3.31	80.29

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ciclosporin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20941-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ciclosporin; Ciclosporinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ciclosporin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ciclosporin	13D26-N07	20941	40	1402057
Caelo	Ciclosporin	13148604	21474	40	1412541
Caelo	Ciclosporin	13148604	21475	40	20130613
Fagron	Ciclosporin	13D26-N07	21671	40	1508429
Caelo	Ciclosporin	173327	24401	40	20180111*
Fagron	Ciclosporin	18G30_B04-354759	24441	40	20181115

Validation samples

A total of 280 317 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 *Ciclosporin*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1619 batches from further 372 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 7 reference samples from the substance/substance group *Ciclosporin*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ciclosporin	12317707	21082	30
Caelo	Ciclosporin	13148604	21474 [†]	20
Caelo	Ciclosporin	13148604	21475 [†]	20
Fagron	Ciclosporin	13D26-N07	21671 [†]	20
Caelo	Ciclosporin	15278907	22966	40
Fagron	Ciclosporin	16C09-B02-325955	23521	30
Caelo	Ciclosporin	171583	23669	40

- 126 692 spectra from a total of 2783 batches from further 781 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*.

- 120 spectra from 52 *Apo-Ident* customers from 53 batches from the substance/substance group *Ciclosporin*.

Supplier	Substance	Batch	Spectra
Fagron	Ciclosporin	12E31-N02	7
Caelo	Ciclosporin	12165603	2
Fagron	Ciclosporin	11K17-N13	1
Caelo	Ciclosporin	12165602	3
Caelo	Ciclosporin	19011301	1
Caelo	Ciclosporin	13031303	1
Fagron	Ciclosporin	13A28-n04	1
Fagron	Ciclosporin	13A28-N04	3
Caelo	Ciclosporin	13A28-N04	4
Fagron	Ciclosporin	25051302	1
Caelo	Ciclosporin	12317702	2
Fagron	Ciclosporin	1103531	1
Fagron	Ciclosporin	13B19-N02	3
Fagron	Ciclosporin	13D26-N07	5
Caelo	Ciclosporin	12317707	4
Caelo	Ciclosporin	13D26-N07	4
Caelo	Ciclosporin	13148606	6
Phönix	Ciclosporin	13D26-N07	1
Fagron	Ciclosporin	13B19N02	2
Fargon	Ciclosporin	13D26-No7	1
VDL	Ciclosporin	13D26-N07	1
Caelo	Ciclosporin	12317703	1
Fagron	Ciclosporin	10J18-N06	1
Fagron	Ciclosporin	13H19N09	1
Fagron	Ciclosporin	13H19-N09	4
Caelo	Ciclosporin	13346808	1
Caelo	Ciclosporin	14A15-No1	1
Caelo	Ciclosporin	13346803	3
Concord Biotech Ltd./ N...	Ciclosporin	14G22-B02-296891	1
Caelo	Ciclosporin	14199104	3
Fagron	Ciclosporin	14G22-B02-296891	5
Fagron	Ciclosporin	14A15-N01	3
Fagron	Ciclosporin	14/18-B02-300180	1
Fagron	Ciclosporin	13414038	1
Caelo	Ciclosporin	15049703	3
Fagron	Ciclosporin	15D23-B05	2
Fagron	Ciclosporin	14718-b02-300180	1
Fagron	Ciclosporin	15D23-B05-307217	1
Caelo	Ciclosporin	15278901	3
Caelo	Ciclosporin	13148604	1
Fagron	Ciclosporin	14a15-n01	1
Fagron	Ciclosporin	15f29-b14-316270	2
Fagron	Ciclosporin	15F29B14316270	1
Fagron	Ciclosporin	15D23-B05-308853	5
Caelo	Ciclosporin	29689114C22B02	1
Caelo	Ciclosporin	15278903	2
Fagron	Ciclosporin	15F29-B14-316270	1
Caelo	Ciclosporin	15278904	3
Caelo	Ciclosporin	15278902	2
Fagron	Ciclosporin	15f29-b14-325654	1
Caelo	Ciclosporin	15278913	1
Caelo	Ciclosporin	17158309	1
Caelo	Ciclosporin	17158303	2
Caelo	Ciclosporin	17158306	1
Caelo	Ciclosporin	17332703	1

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Supplier	Substance	Batch	Spectra
Caelo	Ciclosporin	17332702	2
Caelo	Ciclosporin	18136104	1
Fagron	Ciclosporin	18G30-B04-354759	1

- 78 809 spectra from 565 *Apo-Ident* customers from a total of 26 084 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ciclosporin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ciclosporin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	190	10	126 692
Type C	0	86	34	78 809

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	95.0000 % (> 93.5000 %)
Type C	100.0000 % (> 99.8817 %)	71.6667 % (> 69.1667 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20941	20941	0.00	21.76

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21671	21671	0.00	22.58
21474	21474	0.00	22.00
21475	21474	1.61	22.07
24401	24401	0.00	24.13
24441	20941	6.41	22.05

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ciprofloxacin hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20945-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ciprofloxacin hydrochloride; Ciprofloxacin hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ciprofloxacin hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ciprofloxacin hy...	12B08-N03	20945	40	1401421
Fagron	Ciprofloxacin hy...	14B25-B02	21254	40	20140324

Validation samples

A total of 280317 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 *Ciprofloxacin hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74416 spectra from a total of 1621 batches from further 372 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 *Ciprofloxacin hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ciprofloxacin hydrochloride	15D07-B01-312864	22755	40
Fagron	Ciprofloxacin hydrochloride	15D07-B01-312864	23568	40
Fagron	Ciprofloxacin hydrochloride	16B17-B05-341882	23938	40
Fagron	Ciprofloxacin hydrochloride	17K09-B02-345976	23991	40

- 126732 spectra from a total of 2786 batches from further 781 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 6 *Apo-Ident* customers from 8 batches from the substance/substance group *Ciprofloxacin hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	Ciprofloxacin hydrochloride	14I15-B08-303363	1
Fagron	Ciprofloxacin hydrochloride	14B25-B02-291-783	1
Fagron	Ciprofloxacin hydrochloride	14B25-B02-291783	2

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Supplier	Substance	Batch	Spectra
Fagron	Ciprofloxacin hydrochloride	14/15-B08-303363	1
Fagron	Ciprofloxacin hydrochloride	14I15-B08	1
Fagron	Ciprofloxacin hydrochloride	14I15-B08	1
Fagron	Ciprofloxacin hydrochloride	15D07-B01-312864	1
Caelo	Ciprofloxacin hydrochloride	16B17-B05-324218	1

- 78 920 spectra from 565 *Apo-Ident* customers from a total of 26 129 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ciprofloxacin hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ciprofloxacin hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	160	0	126 732
Type C	0	8	1	78 920

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8818 %)	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
20945	20945	0.00	42.96
21254	20945	8.62	43.45

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Citric acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20019-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Citric acid; Acidum citricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Citric acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Citric acid	11380204	20682	40	20120127
Caelo	Citric acid	12043112	20683	40	20120229
Fagron	Citric acid	12F18-N03	20706	40	20120628
Fagron	Citric acid	13G24-N13	20913	40	20130827
Caelo	Citric acid	13396502	21455	40	20140110
Caelo	Citric acid	13243213	21487	40	20130821
Caelo	Citric acid	160386	22463	40	20160315*

Validation samples

A total of 280 317 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 *Citric acid*. These samples are listed above in the [calibration samples](#) section.
- 74 216 spectra from a total of 1616 batches from further 372 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 [†].

- 500 spectra of 13 reference samples from the substance/substance group *Citric acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citric acid	13396502	21455 [†]	20
Caelo	Citric acid	160386	22463 [†]	20
Caelo	Citric acid	160387	22478	60
Caelo	Citric acid	162086	22620	40
Caelo	Citric acid	162154	22622	40
Caelo	Citric acid	171627	23303	40
Caelo	Citric acid	171626	23421	40
Caelo	Citric acid	171626	23648	40
Caelo	Citric acid	171627	23677	40
Caelo	Citric acid	180976	24034	40
Caelo	Citric acid	181292	24232	40
Caelo	Citric acid	183121	24366	40
Caelo	Citric acid	183071	24367	40

- 126 392 spectra from a total of 2778 batches from further 781 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.

- 1582 spectra from 423 *Apo-Ident* customers from 400 batches from the substance/substance group *Citric acid*.

Supplier	Substance	Batch	Spectra
Gehe	Citric acid	11C24-N03	2
Anzag	Citric acid	10049712	1
Anzag	Citric acid	10049713	1
Euro OTC	Citric acid	1011047-03	2
Caelo	Citric acid	12043105	2
Fagron	Citric acid	11C24-N03	6
Fagron	Citric acid	10G21-N05	2
Caelo	Citric acid	12043118	3
Fagron	Citric acid	11C24-N02	3
Caelo	Citric acid	11159824	1
Eu Rho	Citric acid	L1202001-01	1
Caelo	Citric acid	9158408	1
Gehe	Citric acid	12043111	1
Gehe	Citric acid	11C24-N02	1
Caelo	Citric acid	12043110	4
Caelo	Citric acid	11159801	2
Caelo	Citric acid	12043113	3
Fagron	Citric acid	11K07-N01	7
Caelo	Citric acid	11178303	5
Fagron	Citric acid	20071203	1
Caelo	Citric acid	11K07-N01	1
Caelo	Citric acid	11K11-N02	1
Caelo	Citric acid	11189817	1
Caelo	Citric acid	11380204	5
Euro OTC	Citric acid	L1202001-01	5
Caelo	Citric acid	12043123	6
Noweda	Citric acid	12043110	1
Fagron	Citric acid	700309-0003	2
Fagron	Citric acid	700309-001	1
Fagron	Citric acid	11K07N01	1
Fagron	Citric acid	1151608	2
Gehe	Citric acid	11K07-N01	2
Fagron	Citric acid	12B01-N01	23
Caelo	Citric acid	12156812	4
Caelo	Citric acid	9199105	1
Caelo	Citric acid	12156801	2
Caelo	Citric acid	10049716	1
Caelo	Citric acid	12043120	5
Caelo	Citric acid	12156804	3
Fagron	Citric acid	4810E-01024	1
Caelo	Citric acid	1380208	1
Sanacorp	Citric acid	12156811	1
Finze	Citric acid	12156812	2
Caelo	Citric acid	20060912-3	1
Caelo	Citric acid	20151112-1	1
Caelo	Citric acid	121568704	1
Fagron	Citric acid	12B01-N01	1
Caelo	Citric acid	11C24-N02	1

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Supplier	Substance	Batch	Spectra
Caelo	Citric acid	11066806	1
Caelo	Citric acid	12156803	8
Fagron	Citric acid	1155609	9
Caelo	Citric acid	12043124	3
Caelo	Citric acid	12156811	10
Caelo	Citric acid	713I-01024	1
Caelo	Citric acid	11159821	1
Caelo	Citric acid	11380215	3
Caelo	Citric acid	12B01-N01	5
Caelo	Citric acid	1155609	2
Fagron	Citric acid	12F06-M06	3
Fagron	Citric acid	11K11-N02	2
Caelo	Citric acid	12156827	1
Caelo	Citric acid		3
Caelo	Citric acid	19041305	1
Caelo	Citric acid	19041304	1
Alliance Healthcare	Citric acid	12043123	1
Caelo	Citric acid	12043112	3
Caelo	Citric acid	11380208	1
Fagron	Citric acid	1913A-01024	1
Caelo	Citric acid	13050604	12
Fagron	Citric acid	13804-N02	1
Caesar & Loretz/ Noweda	Citric acid	12156812	1
Caelo	Citric acid	12156818	1
Caelo	Citric acid	12156823	4
Caelo	Citric acid	11159817	1
Phönix	Citric acid	1155609	1
Caelo	Citric acid	13050607	9
Noweda	Citric acid	L1202001-02	1
Caelo	Citric acid	A-040513-1	1
Sanacorp	Citric acid	12156832	1
Fargon	Citric acid	12B01-N01	1
Caelo	Citric acid	13050601	9
Caelo	Citric acid	13050613	16
Caelo	Citric acid	12156832	7
Fagron	Citric acid	12B01-N01	1
Fagron	Citric acid	13A04-N04	12
Sanacorp	Citric acid	1216832	1
Fagron	Citric acid	13A04-N04	1
Phönix Gotha	Citric acid	13050609	1
fargon	Citric acid	13A04-N04	1
Fagron	Citric acid	13A-04-N04	2
Caelo	Citric acid	12156824	5
Sanacorp	Citric acid	12156823	1
Phönix Gotha	Citric acid	13050618	1
Caelo	Citric acid	13050611	6
Phönix Gotha	Citric acid	12B01-N012125/6000	1
Phönix Gotha	Citric acid	12B01-N012028/6000	1
Phönix Gotha	Citric acid	12B01-N011973/6000	1
Fargon	Citric acid	12B01-NN01	1
Caelo	Citric acid	12043119	1
Caelo	Citric acid	13050618	3
Caelo	Citric acid	13050606	2
Fagron	Citric acid	12B01-No1	1
Fagron	Citric acid	13A04-N040019/4900	1
Caelo	Citric acid	12156830	1
Caelo	Citric acid	11380213	1
A.H. 08.06.13 ek: 6,92EUR	Citric acid	13050604	1
Caelo	Citric acid	1305601	1
Fagron	Citric acid	12b01-N01	1

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Supplier	Substance	Batch	Spectra
Noweda	Citric acid	13050601	1
Jungbunzlauer Ladenburg...	Citric acid	1156158	1
Caelo	Citric acid	13050614	7
Caelo	Citric acid	13A04-N04	4
Caelo	Citric acid	2071303	1
Phönix	Citric acid	13A04-N04	1
Jungbunzlauer Ladenburg...	Citric acid	1155609	1
Caelo	Citric acid	13050617	12
Caelo	Citric acid	13050610	5
Caelo	Citric acid	13050623	2
Fagron	Citric acid	12B01N01	1
AHD	Citric acid	13050607	1
Caelo	Citric acid	11C24-N03	1
Sanacorp	Citric acid	12156824	1
Caelo	Citric acid	17071301	1
Fagron	Citric acid	13B04-N01	1
Otto Fischer GmbH	Citric acid	6492061	1
Caelo	Citric acid	13175404	4
Caelo	Citric acid	13050622	7
Caelo	Citric acid	13175402	3
Fagron	Citric acid	12801-N01	1
Caelo	Citric acid	12156822	2
Caelo	Citric acid	13050621	2
Caelo	Citric acid	13175405	4
Caelo	Citric acid	11380217	2
Fagron	Citric acid	26082013B	1
Caelo	Citric acid	10182420	1
Caelo	Citric acid	13050623-3376319052	1
Sanacorp	Citric acid	13050604	1
Caelo	Citric acid	13G24-N13	4
Caelo	Citric acid	27091303	1
Caelo	Citric acid	12175708	3
Fagron	Citric acid	13G04-N05	5
Fagron	Citric acid	13A04N04	1
Caelo	Citric acid	1172673	1
Fagron	Citric acid	probe	1
Caelo	Citric acid	13175411	10
Fagron	Citric acid	13G24-N13	5
Caelo	Citric acid	26111301	1
Caelo	Citric acid	13157404	1
Euro OTC	Citric acid	L130404201	2
Caelo	Citric acid	13175403	13
Caelo	Citric acid	12175711	1
Fargon/Sanacorp	Citric acid		1
Fagron	Citric acid	13G24-N24	12
Fagron	Citric acid	214U-01024	1
Caelo	Citric acid	13050624	1
Fagron	Citric acid	13F12-N01	3
Audor Pharma	Citric acid	PA201	1
Noweda	Citric acid	13050621	1
Gehe	Citric acid	13175404	1
Fagron	Citric acid	700309-0006	1
Caesar/Lorenz	Citric acid	13050610	1
Caelo	Citric acid	L130404202	1
Caelo	Citric acid	13175406	3
Caelo	Citric acid	13175414	2
Fagron	Citric acid	28021404	1
Caelo	Citric acid	28021405	1
Fagron	Citric acid	12175711	1
Caelo	Citric acid	13D29-N02	1

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Supplier	Substance	Batch	Spectra
Phoenix	Citric acid	12b01-N01	1
Fagron	Citric acid	22031401	1
Fagron	Citric acid	13K18-B34-288371	4
Gehe	Citric acid	13175403	1
Phoenix 07.04.2014	Citric acid	13A04-N04	1
Fagron	Citric acid	1714Q1024	1
Caelo	Citric acid	13243201	17
Euro OTC	Citric acid	13175410	1
Caelo	Citric acid	13243202	10
Caelo	Citric acid	13175410	4
Caelo	Citric acid	13175426	4
Caesar & Loretz GmbH	Citric acid	13243201	1
Caelo	Citric acid	13175409	20
Fagron	Citric acid	13G24-N240739/900	1
Fagron	Citric acid	13K18-B34-288372	7
Phoenix	Citric acid	13243202	1
Caelo	Citric acid	12175718	1
Fagron	Citric acid	13K18-B34-291519	5
Caelo	Citric acid	28051401	1
Caelo	Citric acid	13243214	15
Euro OTC	Citric acid	L1202001-02	1
Caelo	Citric acid	13243208	2
Caelo	Citric acid	13243219	4
Fagron	Citric acid	13K18-B34-291521	4
Phönix Gotha	Citric acid	13A04-N040049-100	1
Caesar&loretz,Phoenix	Citric acid	13243201	1
Fagron	Citric acid	13G24-N240029/900	1
Caelo	Citric acid	13243210	8
Alliance Health 03.06.2...	Citric acid	13K18-B34	1
Fagron	Citric acid	100614d	1
Caelo	Citric acid	13243220	2
Caelo	Citric acid	13243221	8
Caelo	Citric acid	160614	1
Euro OTC	Citric acid	13K18-B34	1
Fagron	Citric acid	13K18-B34	5
Caelo	Citric acid	13K18-B34-288372	1
Sanacorp	Citric acid	13243214	1
Caelo	Citric acid	13243217	6
Fagron	Citric acid	13K18-B34-291520	4
Fagron	Citric acid	1172673	6
Sanacorp	Citric acid	40/AKD2	1
Fagron	Citric acid	13K18-B34-291071	4
Caelo	Citric acid	13243224	2
VDL;23.6.14; 2.49EUR	Citric acid	13243213	1
Caelo	Citric acid	12175716	2
Fagron	Citric acid	13K18-B34-291072	2
Caelo	Citric acid	13243213	20
Caelo	Citric acid	13243218	6
Fagron	Citric acid	16072014B	1
GEHE 02.07.2014	Citric acid	13243217	1
Sanacorp	Citric acid	13K18-B34-291072	1
Fagron	Citric acid	1156158	1
Euro OTC	Citric acid	L1304042-02	1
Euro OTC	Citric acid		1
Fischar	Citric acid	6493071	1
	Citric acid	13K18-B34-291523	1
Fagron	Citric acid	13K18-B34-291522	3
Fagron	Citric acid	13K18-B34-293871	2
Caelo	Citric acid	13K18-B34-288371TEST	1
Caelo	Citric acid	12353613	1

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Supplier	Substance	Batch	Spectra
Fagron	Citric acid	11H30-N05	1
Fagron	Citric acid	13F12-N08	1
Caelo	Citric acid	13396504	3
Caesar & Loretz GmbH	Citric acid	13243214	1
Caelo	Citric acid	15091401	1
Caelo	Citric acid	18091409	1
Phoenix	Citric acid	13K18-B34-288372	1
anzag	Citric acid	13175409	1
Fagron	Citric acid	13L18-B39-289347	4
Otto Fischar GmbH&Co. KG	Citric acid	6494061	6
Caelo	Citric acid	13396502	3
Fagron	Citric acid	13k18-B34-288372	1
Caelo	Citric acid	13K18-B34-291520	1
Caelo	Citric acid	13243225	4
Caelo	Citric acid	13396505	2
Bombastus	Citric acid	13396502	1
AHD	Citric acid	13396502	1
Fagron	Citric acid	13K18-B34291522	1
Fagron	Citric acid	13K18-B34-288373	1
Caelo	Citric acid	13K18-B34-291522	1
Fagron	Citric acid	11C24N022869/4250	1
Fagron	Citric acid	13K18-B34-291523	2
Caelo	Citric acid	13243216	11
Fagron	Citric acid	13k18-b34-291522	1
Caelo	Citric acid	14186302	12
Fagron	Citric acid	14E06-B07-293875	3
Fagron	Citric acid	13G24N13	2
Caelo	Citric acid	24021502	1
Caelo	Citric acid	13243005	1
Fagron	Citric acid	13H22-N09	2
Caelo	Citric acid	13031502	1
Euro OTC	Citric acid	1406014-02	1
Caelo	Citric acid	13396506	1
VDL 16.03.15; 2,54EUR	Citric acid	13243201	1
Caelo	Citric acid	1175409	2
Noweda	Citric acid	13243216	1
Euro OTC	Citric acid	13396515	1
Caelo	Citric acid	14041506	1
Phönix	Citric acid	14186312	4
Sanacorb;20.04.15; 7,45EUR	Citric acid	1375410	1
Caelo	Citric acid	14186312	14
Caelo	Citric acid	14186301	19
Caelo	Citric acid	13396515	2
Fagron	Citric acid	14E06-B07293872	1
Caelo	Citric acid	15044903	5
Caelo	Citric acid	13K18-B34	1
Fagron	Citric acid	14E06-B07-293872	3
Caelo	Citric acid	14186313	9
Fagron	Citric acid	13L05-B02-296246	3
Gehe Kassel, 22.05.2015	Citric acid	14E06-B07-293872	1
sanacorp	Citric acid	13396505	1
Fagron	Citric acid	14E06-B07-293890	3
Fagron	Citric acid	14E-06-B07-293890	1
Caelo	Citric acid	14186314	2
Caelo	Citric acid	15044901	6
Fiebig	Citric acid	13243201	1
Caelo	Citric acid	13061502	1
Euro OTC	Citric acid	702260	1
Caelo	Citric acid	133243218	1
Sanacorp	Citric acid	41/AKD4	1

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Supplier	Substance	Batch	Spectra
Caelo	Citric acid	13243222	1
Caelo	Citric acid	14E06-B07	1
Cealo/Gehe	Citric acid	14186301	6
Caelo	Citric acid	15044902	3
Fagron	Citric acid	14b06-b07-293872	1
Caelo	Citric acid	15044905	8
Caelo	Citric acid	1072015B	1
Caelo	Citric acid	15087510	1
Fagron	Citric acid	14G04-B09-293874	10
Caelo	Citric acid	13K18-B34-291523	2
Caelo	Citric acid	14071501	1
Caelo	Citric acid	15124301	8
Fagron	Citric acid	14G04-b09-293876	1
Caeolo/Gehe	Citric acid	15044903	3
Caelo	Citric acid	15063006	4
Euro OTC	Citric acid	L1408011-01	1
Caelo	Citric acid	14G04-B09-293876	4
Fagron	Citric acid	1181765	3
Caelo	Citric acid	15044904	9
Otto Fischer / Sana	Citric acid	6493071	1
Fagron	Citric acid	15044902	1
Fagron	Citric acid	14G04-B09-293876	4
EuRho	Citric acid	L1503027-02	2
Caelo	Citric acid	15063003	19
Fagron	Citric acid	14G04B09293876	1
Caesar & Loretz GmbH	Citric acid	15063003	2
Fagron	Citric acid	11K11-N020444/1975	1
Caelo	Citric acid	1044905	1
Caelo	Citric acid	15063206	17
Fagron	Citric acid	14K05-B04-302816	6
Fagron	Citric acid	14g04-b09293877	1
Caelo	Citric acid	15214301	1
Caelo	Citric acid	15087902	3
Caelo	Citric acid	15063205	2
Euro OTC	Citric acid	L1508013-01	1
Euro OTC	Citric acid	L1503027-02	2
Caelo	Citric acid	15063202	1
Caelo	Citric acid	15063203	10
Caelo	Citric acid	15087903	14
Fagron	Citric acid	13L05-B02-309050	1
Caelo	Citric acid	15063204	8
Klenk	Citric acid	12B01-N01	2
Gehe	Citric acid	15087902	1
Caesar & Loretz	Citric acid	15087904	2
Caelo	Citric acid	15063211	3
Caelo	Citric acid	14G04-B09-293874	2
Caelo	Citric acid	16004701	16
Caelo	Citric acid	1396505	1
Noweda	Citric acid	16004701	1
Caelo	Citric acid	14G04B09293877	1
Caelo	Citric acid	15063218	8
Caelo	Citric acid	16038602	3
Caelo	Citric acid	15088016	1
Euro OTC	Citric acid	L1508013-02	1
Fagron	Citric acid	14G04-B09-293877	7
Caelo	Citric acid	15063213	20
Caelo	Citric acid	1181765	1
Caelo	Citric acid	16004702	21
Caelo	Citric acid	16038604	8
Caelo	Citric acid	15063214	5

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Supplier	Substance	Batch	Spectra
Noweda	Citric acid	15087902	2
Gehe/Fragon	Citric acid	14G04B09293876	1
Caelo	Citric acid	14K05-B04-302815	1
Jenne	Citric acid	15063002	1
Caelo	Citric acid	16004705	3
phönix	Citric acid	16038604	3
fishar	Citric acid	6494061	1
Caelo	Citric acid	16038603	5
Euro OTC	Citric acid	L1408011-02	1
Caelo	Citric acid	15063003-20160615Ma1	1
Caelo	Citric acid	1015U-01024	1
AHD	Citric acid	15063218	1
Caelo	Citric acid	16038704	9
Fagron	Citric acid	14G04-B09-309707	1
Caelo	Citric acid	13243229	1
Fagron	Citric acid	14K05-B04-302815	4
Fragon/Phoenix	Citric acid	14G04-B09-293976	1
Fagron	Citric acid	14k05-b04-302816	1
Ebert & Jacobi 12.07...	Citric acid	1506214	1
Caelo	Citric acid	16004706	13
Caesar&Loretz GmbH	Citric acid	15063213	1
Caelo	Citric acid	1230616	1
Caelo	Citric acid	L1508013-01	1
Caelo	Citric acid	16038701	2
Caelo	Citric acid	16038707	8
Caesar&Loretz GmbH,16.0...	Citric acid	16004706	1
Noweda	Citric acid	15063203	1
Caelo	Citric acid	150632	1
Caelo	Citric acid	15088017	2
Fagron	Citric acid	13L05B02296247	1
Caolo- Noweda	Citric acid	15063213	1
Caelo	Citric acid	15088008	1
Fagron	Citric acid	14G04-B09-309836	3
Caelo	Citric acid	15063217	7
Caelo	Citric acid	16038608	10
Fagron	Citric acid	14K05-B04-302817	2
Caelo	Citric acid	21531	1
Caelo	Citric acid	160607AC	1
Caelo	Citric acid	14G04-B09	1
Caesar & Lorenz GmbH	Citric acid	16004706	1
Caelo	Citric acid	16038606	13
Phoenix 12.12.2016 4,59EUR	Citric acid	1508808	1
12.12.2016 Phoenix 4,59EUR	Citric acid	15088008	1
ALH	Citric acid	L1508013-01	1
Caelo	Citric acid	16038613	6
Lamotte	Citric acid	15063213	1
Caelo	Citric acid	16038710	2
Caelo	Citric acid	7808	1
SanacorpWE:30.01.2017 ...	Citric acid	16038707	1
SanacorpWE:15.02.2017 ...	Citric acid	15063203	1
Cealo/AHD	Citric acid	16038704	1
Caelo	Citric acid	15124303	1
Caelo	Citric acid	xxxxxx	1
Caelo	Citric acid	xxxx	1
Caelo	Citric acid	16038621	10
Caelo	Citric acid	16038708	7
Caelo	Citric acid	8031702	1
Fagron	Citric acid	15G16-B01-330450	6
Fagron	Citric acid	15g16-b01-330450	2
Anzag	Citric acid	6494061	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Citric acid	L1604061-02	2
Fagron	Citric acid	330449	1
Caelo	Citric acid	16038709	4
Caelo	Citric acid	1516Q-01024	1
Caelo	Citric acid	1501-B06-324348	1
Caelo	Citric acid	16038622	3
Gehe	Citric acid	15G16-B01-330450	1
Fagron	Citric acid	15G16-B01330450	1
Caelo	Citric acid	15G16-B01-330450	1
Caelo	Citric acid	2051703	1
Caelo	Citric acid	5315I-01024	1
Fagron	Citric acid	15G16B01330450	1
Fischar	Citric acid	649061	2
Fagron	Citric acid	15G16-B01	2
Caelo	Citric acid	16038607	3
Caelo	Citric acid	1917A-01024	1
Otto Fischar GmbH&Co. KG	Citric acid	6496051	1
Otto Fischar	Citric acid	6494061	1
Caelo	Citric acid	16208607	18
Caelo	Citric acid	16208606	12
Caelo	Citric acid	16208605	12
Fragron/Noweda	Citric acid	15G16-B01-330449	1
Cordes/Noweda	Citric acid	16208607	1
Noweda	Citric acid	16208606	3
Caelo	Citric acid	16208610	7
Fagron	Citric acid	15101-B06-324348	1
Krieger	Citric acid	16038606	1
Caelo	Citric acid	16038614	3
Caelo	Citric acid	170607C/16208605	1
Caelo	Citric acid	2317M-01024	1
Sanacorp	Citric acid	16208608	1
Caelo	Citric acid	16208608	3
phönix	Citric acid	16208608	1
Fagron	Citric acid	15G16-B01-330449	3
Fagron	Citric acid	UJ501	2
Fagron	Citric acid	15G16B01	1
Ebert-Jacobi	Citric acid	16208607	1
Fischer/Noweda	Citric acid	6496091	1
Gehe	Citric acid	16038614	1
Caelo	Citric acid	16208613	8
Fagron	Citric acid	15G16-B01330449	2
Euro OTC	Citric acid	L1609021-01	3
Caelo	Citric acid	16208614	20
Caelo	Citric acid	6071713	1
Fagron	Citric acid	15G16b01	1
Caelo	Citric acid	16215403	1
Caelo	Citric acid	16038713	1
Caelo	Citric acid	26071701	1
Caelo	Citric acid	20170728/Ma1	1
Fagron	Citric acid	16208607	1
Caelo	Citric acid	16208615	1
Caelo	Citric acid	17162701	16
Caelo	Citric acid	1150817/16208614	1
Caelo	Citric acid	3091701	1
Caelo	Citric acid	16208612	9
Caelo	Citric acid	16206813	1
Caelo	Citric acid	2617Q-01024	1
Caelo	Citric acid	16215408	2
Caelo	Citric acid	18111704	1
Caelo	Citric acid	17162702	4

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Supplier	Substance	Batch	Spectra
Caelo	Citric acid	17162603	3
Sanacorp	Citric acid	16208614	1
Caelo	Citric acid	1620610	1
Caelo	Citric acid	16038712	1
Caelo	Citric acid	1716271	1
Fischar	Citric acid	6494061	1
Caelo	Citric acid	L1609021-01	2
Euro OTC	Citric acid	L1609021-02	3
Caelo	Citric acid	17162602	13
GEHE	Citric acid	16208606	1
Caelo	Citric acid	13011801	1
euro / Phoenix 19.02.2018	Citric acid	11609021	1
Euro OTC	Citric acid	11604062-01	1
Caelo	Citric acid	17162601	14
Bombastus	Citric acid	17162601	1
Caelo	Citric acid	16215409	2
Caelo	Citric acid	16215405	1
Caelo	Citric acid	18025801	10
Sanacorp	Citric acid	17162601	1
Caelo	Citric acid	162086055525	1
Cealo/Anzag	Citric acid	16208607	1
Caelo	Citric acid	17329502	2
Caelo	Citric acid	5041802	1
Kehr	Citric acid	17162602	1
Caelo	Citric acid	18025704	8
Caelo	Citric acid	1716262601	1
Caelo	Citric acid	18025702	15
Phönix/Gehe	Citric acid	16208614	1
Caelo	Citric acid	17162604	2
Caelo	Citric acid	17329504	1
Fagron	Citric acid	17E15-B04	2
Caelo	Citric acid	17329503	2
Hepart	Citric acid	16208614	1
Caelo	Citric acid	26051803	1
Caelo	Citric acid	17161601	1
EuRho/Alliance Healthcare	Citric acid	L1609021-02	1
Caelo	Citric acid	18025701	12
Caelo	Citric acid	17329511	2
Caelo	Citric acid	180257045617	1
AHD	Citric acid	17329511	1
Caelo	Citric acid	18025802	4
Caelo	Citric acid	18097603	5
Fagron	Citric acid		1
Fagron	Citric acid	17E15-B04-347169	2
Caelo	Citric acid	18097601	5
Caelo	Citric acid	17329513	2
Sanacorp	Citric acid	18097603	1
Caelo	Citric acid	18097602	2
Caelo	Citric acid	18F25-B02	1
Caelo	Citric acid	18F25-B02-351453	1
Caelo	Citric acid	18097607	2
Caelo	Citric acid	18097606	2
Caelo	Citric acid	18097609	1
Gehe 21-01-2019	Citric acid	18097609	1
Nachtestung-Verlängerung	Citric acid	278/18	1

- 77 347 spectra from 565 *Apo-Ident* customers from a total of 25 744 batches from a further 693

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

Validation results

The validation runs checked whether the substance/substance group *Citric 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 *Citric 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	280	0	74 216
Type B	0	500	0	126 392
Type C	0	1566	16	77 347

The substance/substance group *Citric 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 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.8000 %)
Type C	100.0000 % (> 99.8817 %)	98.9886 % (> 98.7990 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
20682	22463	11.08	42.70
21487	22463	4.13	41.52
20706	22463	11.33	42.52
22463	22463	0.00	39.76
21455	22463	11.92	43.72
20683	22463	1.33	40.41
20913	22463	3.47	39.08

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Citric acid monohydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20012-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citric acid monohydrate; Acidum citricum monohydricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Citric acid monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Citric acid mono...	12D26-N02	20926	40	20120515
Caelo	Citric acid mono...	15185301	22340	40	20150708
Caelo	Citric acid mono...	161865	22617	40	20160706*
Caelo	Citric acid mono...	17085602	23409	40	20170410
Caelo	Citric acid mono...	181305	24222	40	20180606*

Validation samples

A total of 280 317 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 *Citric acid monohydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1618 batches from further 372 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 *Citric acid monohydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citric acid monohydrate	15185301	22340 [†]	20
Caelo	Citric acid monohydrate	161865	23298	40
Hedinger	Citric acid monohydrate	202029	23457	40
Hedinger	Citric acid monohydrate	202029	23458	40

- 126 752 spectra from a total of 2786 batches from further 781 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*.

- 187 spectra from 78 *Apo-Ident* customers from 65 batches from the substance/substance group
Citric acid monohydrate.

Supplier	Substance	Batch	Spectra
Caelo	Citric acid monohydrate	11208133	4
Caelo	Citric acid monohydrate	11208132	3
Caelo	Citric acid monohydrate	1215911	1
Caelo	Citric acid monohydrate	1215907	1
VDL	Citric acid monohydrate	263669	1
Caelo	Citric acid monohydrate	12125907	6
Caelo	Citric acid monohydrate	12125938	1
Phönix	Citric acid monohydrate	10111503	1
Caelo	Citric acid monohydrate	13069104	6
Sanacorp	Citric acid monohydrate	1215937	1
Caelo	Citric acid monohydrate	1212937	1
Caelo	Citric acid monohydrate	12125937	3
Caesar &Loretz GmbH	Citric acid monohydrate	12125937	1
Caelo	Citric acid monohydrate	12125904	2
Caelo	Citric acid monohydrate	13069106	3
Caelo	Citric acid monohydrate	13069111	3
Fiebig28.08.13 EK6,60	Citric acid monohydrate	13069111	1
Caelo	Citric acid monohydrate	13069113	2
Caelo	Citric acid monohydrate	13069110	4
Bombastus	Citric acid monohydrate	259437	1
Caelo	Citric acid monohydrate	13069124	4
Caelo	Citric acid monohydrate	13069128	3
Caelo	Citric acid monohydrate	13069105	2
Caelo	Citric acid monohydrate	13069125	2
Caelo	Citric acid monohydrate	14038401	6
Caelo	Citric acid monohydrate	13069129	4
Caelo	Citric acid monohydrate	13069133	5
Caelo	Citric acid monohydrate	14038403	7
Sanacaorp	Citric acid monohydrate	14038401	2
Caelo	Citric acid monohydrate	14311808	4
Caelo	Citric acid monohydrate	14311807	2
Caelo	Citric acid monohydrate	13069130	1
Caelo	Citric acid monohydrate	14311812	4
Caelo	Citric acid monohydrate	15087502	2
Caelo	Citric acid monohydrate	15087503	2
Caelo	Citric acid monohydrate	15087509	8
Caelo	Citric acid monohydrate	13069103	1
Caelo	Citric acid monohydrate	15087510	2
Caelo	Citric acid monohydrate	14311813	1
Caelo	Citric acid monohydrate	15087512	1
Caelo	Citric acid monohydrate	15185304	10
Caelo	Citric acid monohydrate	2515Q-02959	1
Caelo	Citric acid monohydrate	15185302	10
Krieger	Citric acid monohydrate	613001-1-P	1
Caelo	Citric acid monohydrate	15185301	2
Caelo	Citric acid monohydrate	15185309	2
Caelo	Citric acid monohydrate	15185317	1
Caelo	Citric acid monohydrate	15185314	4
Caelo	Citric acid monohydrate	15185316	5
Ebert 17.08.16	Citric acid monohydrate	15185314	1
Caelo	Citric acid monohydrate	15185321	3
Caelo	Citric acid monohydrate	15185320	2
Caelo	Citric acid monohydrate	16186501	2
Phönix	Citric acid monohydrate	1403/3	1
Caelo	Citric acid monohydrate	16186502	5
Caelo	Citric acid monohydrate	14071701	1
Hedinger	Citric acid monohydrate	202029	2

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Supplier	Substance	Batch	Spectra
Bombastus	Citric acid monohydrate	309344	2
Caelo	Citric acid monohydrate	16186508	4
Caelo	Citric acid monohydrate	17085603	1
Hedinger/Phönix	Citric acid monohydrate	202029	1
Bombastus	Citric acid monohydrate	309650	1
Caelo	Citric acid monohydrate	17085602	6
Caelo	Citric acid monohydrate	sjdfksjfdkl	1
Caelo	Citric acid monohydrate	161865001	1
Bombastus	Citric acid monohydrate	70620101	1
Caelo	Citric acid monohydrate	17329804	3
Caelo	Citric acid monohydrate	17085607	2
Caelo	Citric acid monohydrate	17329807	1
Caelo	Citric acid monohydrate	17329801	1

- 78 742 spectra from 565 *Apo-Ident* customers from a total of 26 074 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Citric acid monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citric acid monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	140	0	126 752
Type C	0	175	12	78 742

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.8817 %)	93.5829 % (> 91.9786 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
20926	22617	10.30	36.51
22340	22617	2.66	36.90
22617	22617	0.00	36.42
23409	22617	11.04	37.26
24222	24222	0.00	41.73

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Citrulline**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21095-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Citrulline; Citrullinum; L-citrulline

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Citrulline*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Citrulline	1310015-01	21095	40	20131120
Euro OTC	Citrulline	1403021-01	21565	40	1411031
Euro OTC	Citrulline	1506014	21828	40	20150624*
Euro OTC	Citrulline	1604038	22560	40	20160523*
Euro OTC	Citrulline	1703036	23175	40	20170418*
Euro OTC	Citrulline	1811028	24348	40	20181127*

Validation samples

A total of 280 317 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 *Citrulline*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 [†].

- 239 spectra of 7 reference samples from the substance/substance group *Citrulline*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Citrulline	1403021-01	21565 [†]	19
Euro OTC	Citrulline	1506014	21828 [†]	20
Euro OTC	Citrulline	1609013	22866	40
Euro OTC	Citrulline	1707003	23538	40
Fagron	Citrulline	16D11-B02-326797	23567	40
Euro OTC	Citrulline	1710039	23913	40
Euro OTC	Citrulline	1805028	24117	40

- 126 653 spectra from a total of 2782 batches from further 781 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*.

- 3 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Citrulline*.

Supplier	Substance	Batch	Spectra
Gall-Pharma GmbH	Citrulline		1
Euro OTC	Citrulline	16040038-01	1
Gall-Pharma GmbH/Noweda	Citrulline		1

- 78 926 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Citrulline* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrulline* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	239	0	126 653
Type C	0	3	0	78 926

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.4895 %)
Type C	100.0000 % (> 99.8821 %)	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
22560	22560	0.00	47.53
23175	23175	0.00	48.19
21095	21565	7.80	44.01
21565	21565	0.00	43.15
24348	24348	0.00	45.56
21828	21828	0.00	46.22

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Clindamycin hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20214-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Clindamycin hydrochloride; Clindamycini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Clindamycin hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Clindamycin hydr...	1111058-01	20757	80	20120516
Fagron	Clindamycin hydr...	13G24-N09	21224	40	1412075
Euro OTC	Clindamycin hydr...	1511004	21996	40	20151123*
Euro OTC	Clindamycin hydr...	1510038	22224	40	20151120*
Caelo	Clindamycin hydr...	15392809	22958	40	20151204

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Clindamycin hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74256 spectra from a total of 1618 batches from further 372 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 *Clindamycin hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Clindamycin hydrochloride	1401041-01	21239	40
Euro OTC	Clindamycin hydrochloride	1511004	21996 [†]	20
Euro OTC	Clindamycin hydrochloride	1510038	22224 [†]	20
Caelo	Clindamycin hydrochloride	15392817	23245	40
Fagron	Clindamycin hydrochloride	16D05-B08-332106	23264	40
Caelo	Clindamycin hydrochloride	153928	23365	40
Caelo	Clindamycin hydrochloride	172093	23681	40
Euro OTC	Clindamycin hydrochloride	1710013	23769	40
Euro OTC	Clindamycin hydrochloride	1811003	24336	40

- 126572 spectra from a total of 2780 batches from further 781 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.

- 239 spectra from 98 *Apo-Ident* customers from 118 batches from the substance/substance group *Clindamycin hydrochloride*.

Supplier	Substance	Batch	Spectra
Euro OTC	Clindamycin hydrochloride	2908019V-03	4
Gehe	Clindamycin hydrochloride	11E12-N02	1
Gehe	Clindamycin hydrochloride	11K04-N12	1
Gehe	Clindamycin hydrochloride	700168-0002	1
Euro OTC	Clindamycin hydrochloride	1111058-01	5
Fargon	Clindamycin hydrochloride	11L20-No5	1
Noweda	Clindamycin hydrochloride	2908019V-03	1
Euro OTC	Clindamycin hydrochloride	111158-01	1
Caelo	Clindamycin hydrochloride	11K04-N12	1
Fargon	Clindamycin hydrochloride	12F19-N07	3
Europharm/Otto	Clindamycin hydrochloride	1111058-01	1
Fargon	Clindamycin hydrochloride	12C19-N06	1
Caelo	Clindamycin hydrochloride		1
Gehe	Clindamycin hydrochloride	13a22-n01	1
Fargon	Clindamycin hydrochloride	13A22-N01	6
Cealo	Clindamycin hydrochloride	1111058-01	1
Fargon	Clindamycin hydrochloride	P003-WS10100301	1
Caelo	Clindamycin hydrochloride	P-003-WS10100301	1
Euro OTC	Clindamycin hydrochloride	1111058-02	1
Fargon	Clindamycin hydrochloride	13C15-N06	1
AHD	Clindamycin hydrochloride	130402X5	1
Euro OTC	Clindamycin hydrochloride	1111058-03	3
Gehe	Clindamycin hydrochloride	13A22-N01	1
Fargon	Clindamycin hydrochloride	13G24-N09	7
Caelo	Clindamycin hydrochloride	1111058-03	1
Euro OTC	Clindamycin hydrochloride	1401041-01	11
Fargon	Clindamycin hydrochloride	13G24N09	1
Fargon	Clindamycin hydrochloride	13J03-B02-288655	1
Euro OTC	Clindamycin hydrochloride	25071401	1
Caelo	Clindamycin hydrochloride	13G24-N09	1
Fargon	Clindamycin hydrochloride	P003WS13091401	1
Caelo	Clindamycin hydrochloride	1401041-01	2
Fargon	Clindamycin hydrochloride	13J03B02288654	1
Fargon	Clindamycin hydrochloride	2714Q-03534	1
Fargon	Clindamycin hydrochloride	13J03-B02	1
Euro OTC	Clindamycin hydrochloride	130709X8	2
Euro OTC	Clindamycin hydrochloride	SCHE1107035	1
Phönix	Clindamycin hydrochloride	12H30-N04	1
Fargon	Clindamycin hydrochloride	13J03-B02288654	1
EuRho	Clindamycin hydrochloride	1401041-01	1
Euro OTC	Clindamycin hydrochloride	1401041-02	6
Fargon	Clindamycin hydrochloride	13J03-B02-288654	3
Euro OTC	Clindamycin hydrochloride	140104101	1
Euro OTC	Clindamycin hydrochloride	T03-05/1401041-01	1
Euro OTC	Clindamycin hydrochloride	813M-03534	1
Euro OTC	Clindamycin hydrochloride	140104102	3
Fargon	Clindamycin hydrochloride	13j03-B02-288653	1
Euro OTC	Clindamycin hydrochloride	700168	1
Fargon	Clindamycin hydrochloride	111105803	1
Fargon	Clindamycin hydrochloride	14K04-B05-304995	1
Caelo	Clindamycin hydrochloride	140104102	1
Fargon	Clindamycin hydrochloride	14D23-B03	1

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Supplier	Substance	Batch	Spectra
Fagron	Clindamycin hydrochloride	14K04-B05-304996	1
Caelo	Clindamycin hydrochloride	14K04B05309851	1
Fagron	Clindamycin hydrochloride	14K04-B05-309851	1
Fagron	Clindamycin hydrochloride	15E06-B12-310472	1
Fagron	Clindamycin hydrochloride	15E06-B12-313089	2
Fagron	Clindamycin hydrochloride	15E06-B12-311886	2
Fagron	Clindamycin hydrochloride	14K04-B05-313090	1
Euro OTC	Clindamycin hydrochloride	1510038-01	17
Euro OTC	Clindamycin hydrochloride	1401401-01	1
Fagron	Clindamycin hydrochloride	15E06-B12-314066	1
Caelo	Clindamycin hydrochloride	15E06-B12-310472	1
Euro/Gehe16.03.16	Clindamycin hydrochloride	1510038-01	1
Caelo	Clindamycin hydrochloride	151003801	2
Euro OTC	Clindamycin hydrochloride	1511004-01	13
Fagron	Clindamycin hydrochloride	15L22-B03-316670	1
Caelo	Clindamycin hydrochloride	15392802	1
Phönix	Clindamycin hydrochloride	15392803	1
Euro OTC	Clindamycin hydrochloride	1510030-01	1
Fagron	Clindamycin hydrochloride	1010616	1
Caelo	Clindamycin hydrochloride	1511004-01	1
Fagron	Clindamycin hydrochloride	15L22-B03-318787	1
Euro OTC	Clindamycin hydrochloride	151100401	2
Caelo	Clindamycin hydrochloride	15L22-B03-318788	1
Caelo	Clindamycin hydrochloride	15392807	1
Caelo	Clindamycin hydrochloride	15392811	2
Caelo/AHD	Clindamycin hydrochloride	16D05-B08-325088	1
Caelo	Clindamycin hydrochloride	15392805	1
Fagron	Clindamycin hydrochloride	16D05-B08-321572	1
Fagron	Clindamycin hydrochloride	16D05-B08-320327	2
Fagron	Clindamycin hydrochloride	1600324C	1
Fargon	Clindamycin hydrochloride	16D05-B08-320327	1
Fagron	Clindamycin hydrochloride	16D05-B08-325088	3
Fagron	Clindamycin hydrochloride	16D05-B08-328259	1
Euro OTC	Clindamycin hydrochloride	16D05-B08-328259	1
Fagron	Clindamycin hydrochloride	16D05-B08	2
Euro OTC	Clindamycin hydrochloride	1510038-02	3
Euro OTC	Clindamycin hydrochloride	150901B	1
Caelo	Clindamycin hydrochloride	1511004-02	1
Caelo	Clindamycin hydrochloride	15392815	2
Fagron	Clindamycin hydrochloride	16D05-B08-323321	1
Fagron	Clindamycin hydrochloride	16D05-B08-327127	1
Fagron	Clindamycin hydrochloride	16D05-B08-332105	1
Anzag	Clindamycin hydrochloride	15392815	1
Fagron	Clindamycin hydrochloride	16D05-B08-330624	1
Sanacorp	Clindamycin hydrochloride	1511004-03	1
Phoenix	Clindamycin hydrochloride	16D05-B08-327127	1
Caelo	Clindamycin hydrochloride	1511004-03	1
Fagron	Clindamycin hydrochloride	16D05-B08-328260	1
Fagron	Clindamycin hydrochloride	16D05-B08-325087	1
Euro OTC	Clindamycin hydrochloride	4988149	1
Caelo	Clindamycin hydrochloride	15392814	1
Sanacorp	Clindamycin hydrochloride	16D05-B08-332106	1
Euro OTC	Clindamycin hydrochloride	1511004-02	3
Caelo	Clindamycin hydrochloride	15392804	1
Fagron	Clindamycin hydrochloride	16D05-B08-332106	1
Fagron	Clindamycin hydrochloride	16d05-b08-332107	1
Fagron	Clindamycin hydrochloride	16d05-b08-325089	1
Caelo	Clindamycin hydrochloride	15392817	2
Caelo	Clindamycin hydrochloride	15392819	1
phönix	Clindamycin hydrochloride	15392820	1

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Supplier	Substance	Batch	Spectra
noweda	Clindamycin hydrochloride	1511004-03	1
Euro OTC	Clindamycin hydrochloride	1710013-01	10
Caelo	Clindamycin hydrochloride	15392818	1
Euro OTC	Clindamycin hydrochloride	1511004-002	1
Fagron	Clindamycin hydrochloride	16H03-B02-334345	1
Fagron	Clindamycin hydrochloride	16H03-B02-338803	2
Caelo	Clindamycin hydrochloride	15392822	1
Caelo	Clindamycin hydrochloride	16H03-B03-334345	1
Caelo	Clindamycin hydrochloride	16H03-B02	1
Fagron	Clindamycin hydrochloride	18041801	1
Sanacorp	Clindamycin hydrochloride	16H03-B02-341602	1
Fagron	Clindamycin hydrochloride	16H03-B02	1
Sanacorp	Clindamycin hydrochloride	16H03-B02-339275	1
Euro OTC	Clindamycin hydrochloride	171001301	1
Euro OTC	Clindamycin hydrochloride	8061801	1
Bombastus	Clindamycin hydrochloride	1710013-01	1
Fagron	Clindamycin hydrochloride	16H03-B02-336706	1
Fagron	Clindamycin hydrochloride	18A18-B08-346107	1
Fagron	Clindamycin hydrochloride	18A18-B08	1
Fagron	Clindamycin hydrochloride	18A18-B08-346106	1
Fagron	Clindamycin hydrochloride	18D11-B01-349677	1
Fagron	Clindamycin hydrochloride	18D11-B01	1
Caelo	Clindamycin hydrochloride	10809406	1
Caelo	Clindamycin hydrochloride	160712C	1
Sanacorp	Clindamycin hydrochloride	18A18-B08-347483	1
Caelo	Clindamycin hydrochloride	17001301	1
Caelo	Clindamycin hydrochloride	1811003-01	2
Sanacorp	Clindamycin hydrochloride	K-171219B	1
Sanacorp	Clindamycin hydrochloride	18D11-B01-352732	1
Caelo	Clindamycin hydrochloride	18009413	1

- 78 690 spectra from 565 *Apo-Ident* customers from a total of 26 021 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Clindamycin hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clindamycin hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	320	0	126 572
Type C	0	229	10	78 690

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.8817 %)	95.8159 % (> 94.5607 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21224	21224	0.00	18.79
21996	21996	0.00	19.92
22224	22224	0.00	19.22
22958	21996	2.65	20.56
20757	21996	3.62	21.36

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Clindamycin-2-dihydrogen phosphate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21063-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Clindamycin-2-dihydrogen phosphate; Clindamycini phosphas

Special notes

When selecting the *Clindamycin-2-dihydrogen phosphate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Clindamycin-2-dihydrogen phosphate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clindamycin-2-di...	13166605	21063	40	1403485
Caelo	Clindamycin-2-di...	13166605	21116	40	20130624
Caelo	Clindamycin-2-di...	15435801	22312	40	AR-16-FG-009129-01
Caelo	Clindamycin-2-di...	163265	23055	40	20161214*
Caelo	Clindamycin-2-di...	16326504	23586	40	AR-17-FG-022557-01

Validation samples

A total of 280 317 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 *Clindamycin-2-dihydrogen phosphate*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1619 batches from further 372 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 [†].

- 280 spectra of 6 reference samples from the substance/substance group *Clindamycin-2-dihydrogen phosphate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clindamycin-2-dihydrogen pho...	14257305	21798	60
Caelo	Clindamycin-2-dihydrogen pho...	15435801	22312 [†]	20
Caelo	Clindamycin-2-dihydrogen pho...	172964	24047	40
Caelo	Clindamycin-2-dihydrogen pho...	14257305	21798SI	60
Caelo	Clindamycin-2-dihydrogen pho...	15435801	22312SI	60
Caelo	Clindamycin-2-dihydrogen pho...	163265	23055SI	40

- 126 612 spectra from a total of 2785 batches from further 781 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*.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Clindamycin-2-dihydrogen phosphate*.

Supplier	Substance	Batch	Spectra
Caelo	Clindamycin-2-dihydrogen pho...	14257305	1
Caelo	Clindamycin-2-dihydrogen pho...	17344101	1

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Clindamycin-2-dihydrogen phosphate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clindamycin-2-dihydrogen phosphate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	143	137	126 612
Type C	0	2	0	78 927

The substance/substance group *Clindamycin-2-dihydrogen phosphate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	51.0714 % (> 50.0000 %)
Type C	100.0000 % (> 99.8823 %)	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
23055	23055	0.00	22.22
21063	21063	0.00	21.92
21116	21063	0.84	24.03
22312	22312	0.00	35.43
23586	23586	0.00	27.74

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Clioquinol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20095-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Clioquinol; Clioquinolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Clioquinol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clioquinol	11304120	20895	40	20111208
Fagron	Clioquinol	13I26-N15	21236	40	20131028
Euro OTC	Clioquinol	1309009-02	21246	40	AR-15-FG-009542-01
Fagron	Clioquinol	14I11-B03-300049	21913	40	20140926
Euro OTC	Clioquinol	1509038	21944	40	20151009*
Fagron	Clioquinol	14I11-B03-300049	21972	40	20140926
Caelo	Clioquinol	163072	23047	40	20161202*

Validation samples

A total of 280317 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 *Clioquinol*. These samples are listed above in the [calibration samples](#) section.
- 74216 spectra from a total of 1617 batches from further 372 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 [†].

- 260 spectra of 8 reference samples from the substance/substance group *Clioquinol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clioquinol	13114413	21308	40
Fagron	Clioquinol	14I11-B03-300049	21913 [†]	20
Euro OTC	Clioquinol	1509038	21944 [†]	20
Fagron	Clioquinol	14I11-B03-300049	21972 [†]	20
Caelo	Clioquinol	16307206	22960	40
Euro OTC	Clioquinol	1612020	22985	40
Caelo	Clioquinol	172046	23633	40
Caelo	Clioquinol	182782	24374	40

- 126632 spectra from a total of 2782 batches from further 781 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.

- 648 spectra from 293 *Apo-Ident* customers from 184 batches from the substance/substance group *Clioquinol*.

Supplier	Substance	Batch	Spectra
Euro OTC	Clioquinol	1102022-02	3
Euro OTC	Clioquinol	1102022-01	2
Caelo	Clioquinol	10341605	4
Caelo	Clioquinol	10341601	2
Euro OTC	Clioquinol	2507212562	1
Caelo	Clioquinol	1201034-01	1
Caelo	Clioquinol	11304102	7
Fagron	Clioquinol	11K21-N18	4
Euro OTC	Clioquinol		1
Fagron	Clioquinol	11G20-N09	1
Euro OTC	Clioquinol	1201034-01	5
Fagron	Clioquinol	1005090024	1
Euro OTC	Clioquinol	1201034-02	7
Caelo	Clioquinol	11304107	5
Sanacorp	Clioquinol	11304111	1
Noweda	Clioquinol	11304111	1
Caelo	Clioquinol	11304111	2
Caelo	Clioquinol	11304112	6
Noweda	Clioquinol	1201034-02	2
Noweda	Clioquinol	11304107	1
Caelo	Clioquinol	5031302	1
Fagron	Clioquinol	12L04-N08	7
Fagron	Clioquinol	12F20-N05	3
Sanacorp	Clioquinol	1201034-01	1
Fagron	Clioquinol	11304112	1
Phönix	Clioquinol	1102022-02	3
Noweda	Clioquinol	10057206	1
Caelo	Clioquinol	11304113	4
Caelo	Clioquinol	10341608	1
Caelo	Clioquinol	1130312	1
Caelo	Clioquinol	11304105	3
Anzag	Clioquinol	12L04-N08	1
Caelo	Clioquinol	11304116	3
Caelo	Clioquinol	13A29-N07	1
Caelo	Clioquinol	11304117	10
Caelo	Clioquinol	12L04-N08	2
Caelo	Clioquinol	11304103	1
Fagron	Clioquinol	13A29-N07	7
Caelo	Clioquinol	12F20-N05	1
Caelo	Clioquinol	13114404	2
Caelo	Clioquinol	11304120	12
Caelo	Clioquinol	11304119	3
Caelo	Clioquinol	3513I-02562	1
Caelo	Clioquinol	3713A2562	1
Caelo	Clioquinol	1201034-02	2
Caelo	Clioquinol	11304109	1
Caelo	Clioquinol	130114-02	1
EuRho	Clioquinol	1201034-02	1
Euro OTC	Clioquinol	1301014-01	2
Fagron	Clioquinol	13A29-N07-3398310111	1
Fagron	Clioquinol	13D15-N01	8
Klenk	Clioquinol	11304120	1
Euro OTC	Clioquinol	1301014-02	5
Caelo	Clioquinol	4613E2562	1

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Supplier	Substance	Batch	Spectra
Nachprüfung	Clioquinol	3021U-02562	1
Fagron	Clioquinol	7D20-N03	1
Caelo	Clioquinol	11304124	13
Fagron	Clioquinol	13DS15-N01	1
Fagron	Clioquinol	11304120	1
Euro OTC	Clioquinol	1309009-01	6
Caelo	Clioquinol	5213A2562	1
Phönix Gotha	Clioquinol	11304124	1
Euro OTC	Clioquinol	PC86	1
Caelo	Clioquinol	13114406	1
Fagron	Clioquinol	13F12-N20	2
Caelo	Clioquinol	13114408	3
Fagron	Clioquinol	13F12-N200463480	1
Sanacorp	Clioquinol	11304124	1
Caelo	Clioquinol	13114413	10
Axyntis Group	Clioquinol	1301014-02	1
Caelo	Clioquinol	1214I02562	1
Phoenix	Clioquinol	11304119	1
Caelo	Clioquinol	3041409	1
Fagron	Clioquinol	28031401	1
Caelo/Sanacorp	Clioquinol	1309009-01	1
Fagron	Clioquinol	1205110014	1
VDL	Clioquinol	131144131	1
Noweda	Clioquinol	1309009-01	1
Caelo	Clioquinol	13114410	2
Fagron	Clioquinol	13I26N15	1
Fagron	Clioquinol	14052014C	1
EuRho	Clioquinol	1309009-02	1
Fagron	Clioquinol	2014Q2562	1
Caelo	Clioquinol	10341510	1
Phoenix	Clioquinol	13114408	2
Caelo	Clioquinol	13114415	3
Fagron	Clioquinol	13I26-N15	4
Fagron	Clioquinol	2514U2562	1
Caelo	Clioquinol	13114417	7
Euro OTC	Clioquinol	1301014	1
Fagron	Clioquinol	1326-N15	3
Fagron	Clioquinol	13114417	1
Euro OTC	Clioquinol	1309009-02	10
Phoenix	Clioquinol	13114417	1
Phönix	Clioquinol	14C21-B08	1
GEHE 04.08.2014	Clioquinol	13114418	1
Caelo	Clioquinol	1309009-02	1
Euro OTC	Clioquinol	130900902	1
Caelo	Clioquinol	13114418	5
anzag	Clioquinol	13114418	1
Phönix	Clioquinol	13114417	1
Euro OTC	Clioquinol	1303009-02	1
Fagron	Clioquinol	13/26-N15	2
Phönix	Clioquinol	1309009-02	1
Fagron	Clioquinol	14C21-B06-293104	6
Caelo	Clioquinol	13114422	7
Caelo	Clioquinol	5089	1
Caelo	Clioquinol	13114424	10
Fagron	Clioquinol	13114424	1
Fagron	Clioquinol	14-C21-B06-293132	1
Euro OTC	Clioquinol	13010104-03	1
Caelo	Clioquinol	13114423	10
Fagron	Clioquinol	14c21B06293104	1
Fagron	Clioquinol	14C21-B06-293132	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Clioquinol	13114422	1
Euro OTC	Clioquinol	1305070109	1
Caelo	Clioquinol	14C21-B06-293104	1
Fagron	Clioquinol	1305120028	1
Euro OTC	Clioquinol	140903101	1
Caelo	Clioquinol	16021505	1
Caelo	Clioquinol	13114421	1
Euro OTC	Clioquinol	1409031-01	5
Fagron	Clioquinol	14C21-B08	1
Phönix	Clioquinol	14C21-B06	2
Fagron	Clioquinol	14C21-B06	2
Euro OTC	Clioquinol	1409031-02	9
Euro OTC	Clioquinol	1213A-02562	1
Fagron	Clioquinol	14I11-B03	2
Caelo	Clioquinol	13114427	2
Caelo	Clioquinol	14359102	8
Sanacorp	Clioquinol	8/AKD4	1
Fiebig	Clioquinol	1409031-02	2
Caelo	Clioquinol	1405080036	1
Fagron	Clioquinol	1309009-01	1
Fagron	Clioquinol	14I11-B03-300049	4
Axyntis Group	Clioquinol	1301014-03	1
Fagron	Clioquinol	14C21806293104	1
Fagron	Clioquinol	14C21-B06-297159	3
Fagron	Clioquinol	14/11-B03-300049	3
Caelo	Clioquinol	1405080031	1
Fagron	Clioquinol	1411-B03-300049	2
Fagron	Clioquinol	1411B03300049	1
Noweda	Clioquinol	14359103	1
Caelo	Clioquinol	14359103	9
Unisan	Clioquinol	14/11-B03	1
Fagron	Clioquinol		1
Euro OTC	Clioquinol	14090131-02	1
Fagron	Clioquinol	14I11-B03-3000049	1
Fagron	Clioquinol	14I11-B03-309048	2
Caelo	Clioquinol	14359111	12
caesar&loretz,Phönix	Clioquinol	14359111	1
Nachprüfung	Clioquinol	13L26-N15	2
Euro OTC	Clioquinol	1509038-31	1
Euro	Clioquinol	1509038-01	2
Fagron	Clioquinol	14I11-B03-309181	2
Cael Sanacorp 05.02.2016	Clioquinol	14359103	1
Caelo	Clioquinol	14359112	13
Euro OTC	Clioquinol	1509038-01	10
Fagron	Clioquinol	14/11-B03-309181	1
Euro OTC	Clioquinol	150903-01	1
Caelo	Clioquinol	14359117	2
Caelo	Clioquinol	1509038-01	1
Caelo	Clioquinol	14359118	9
Caelo	Clioquinol	14359113	1
Caelo	Clioquinol	14/-B03-309181	1
Euro OTC	Clioquinol	1509038-02	22
Euro OTC	Clioquinol	1509038	2
Caelo	Clioquinol	144359111	1
Caelo	Clioquinol	14/11-B03-309181	1
Bombastus	Clioquinol	14359118	1
Caelo	Clioquinol	14359120	6
wepa/Sanaco	Clioquinol	1439118	1
Caelo	Clioquinol	14/11-BG03-309181	1
Caelo	Clioquinol	14359119	3

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Supplier	Substance	Batch	Spectra
Fagron	Clioquinol	15L30-B05-314974	6
Fagron	Clioquinol	14359118	1
Caelo	Clioquinol	4214Q-02562	1
Caelo	Clioquinol	1509038-02	2
Noweda	Clioquinol	14359120	1
Caelo	Clioquinol	14353120	1
Caolo- Noweda	Clioquinol	14359118	1
Fagron	Clioquinol	1505120044	1
Apo-ident	Clioquinol	1509038-02	1
Caelo	Clioquinol	160916CL	1
Caelo	Clioquinol	15L30-B05-314974	1
Euro OTC	Clioquinol	14359120	1
Fagron	Clioquinol	14111-B03-300049	1
Fagron	Clioquinol	3916U-02562	1
Euro OTC	Clioquinol	150903802	1
Fagron	Clioquinol	15L30-B05-319616	2
Fagron	Clioquinol	15L30-B05	1
Euro OTC	Clioquinol	1509038-03	10
GEHE	Clioquinol	1509038-03	1
EURO / Sanacorp	Clioquinol	150903802	1
Fagron	Clioquinol	15L30-B05-321899	3
Caelo	Clioquinol	16307205	8
Fagron	Clioquinol	16J18-B04-328511	1
Caelo	Clioquinol	16307206	15
Caelo	Clioquinol	16307204	1
Fagron	Clioquinol	16/18-b04-328511	1
Fagron	Clioquinol	15L30-321899	1
Fagron	Clioquinol	15L30-B05-321899	1
Fagron	Clioquinol	16J18-B04-328520	1
Caelo	Clioquinol	14359116	1
Caelo	Clioquinol	16307207	12
Fagron	Clioquinol	14/11-Bo3	1
Caelo	Clioquinol	1509038-03	3
Fagron	Clioquinol	16J18-B04-329141	2
Gehe	Clioquinol	1509038-03	1
Caelo	Clioquinol	16307208	4
Caelo	Clioquinol	16118-B04-329141	1
Caelo	Clioquinol	16307209	1
phönix	Clioquinol		1
Caelo	Clioquinol	16307203	2
GEHE	Clioquinol	1509038-02	1
Caelo	Clioquinol	163072	1
Fagron	Clioquinol	16J18-B04	2
Sanacorp	Clioquinol	16J18-B04-328511	1
Caelo	Clioquinol	170926CL/16307208	1
Caelo	Clioquinol	150903803	1
Fagron	Clioquinol	16J18-B04-32914	1
Caelo	Clioquinol	16J18-B04-328520	1
Caelo	Clioquinol	16307211	5
Euro OTC	Clioquinol	1612020-01	10
Caelo	Clioquinol	16307214	8
EuRho	Clioquinol	1612020-01	1
Caelo	Clioquinol	16307213	1
Caelo	Clioquinol	16307210	2
Noweda	Clioquinol	16307208	1
Euro OTC	Clioquinol	2195137	1
Fagron	Clioquinol	1605100008	1
Caelo	Clioquinol	1612020-01	1
Phönix	Clioquinol	16718b04332852	1
Caelo	Clioquinol	180127C/16307215	1

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Supplier	Substance	Batch	Spectra
Caelo	Clioquinol	16307215	3
Caelo	Clioquinol	16122020-01	1
EuRho	Clioquinol	161202001	1
Caelo	Clioquinol	16307216	4
Caelo	Clioquinol	17204603	6
Caelo	Clioquinol	17204601	2
Caelo	Clioquinol	18011502	13
Fagron	Clioquinol	16J18B04	1
Fagron	Clioquinol	16/18-B04-332852	1
Fagron	Clioquinol	18B05-B07-345483	1
Caelo	Clioquinol	18011516	3
Caelo	Clioquinol	1509038-OTC-Pharma	1

- 78 281 spectra from 565 *Apo-Ident* customers from a total of 25 953 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Clioquinol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clioquinol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 216
Type B	0	260	0	126 632
Type C	0	541	107	78 281

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.8817 %)	83.4877 % (> 83.0247 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20895	21246	3.45	64.87
21236	21246	3.39	64.25
21246	21246	0.00	65.93
21913	21944	2.38	65.79
21944	21944	0.00	65.81
21972	21944	3.52	64.53
23047	23047	0.00	63.27

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Clobetasol propionate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20030-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Clobetasol propionate; Clobetasoli propionas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Clobetasol propionate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clobetasol propi...	13134705	21092	80	AR-15-FG-005328-01
Caelo	Clobetasol propi...	13269505	21473	40	AR-15-FG-000622-02
Euro OTC	Clobetasol propi...	1211021-04	21611	40	1605044
Caelo	Clobetasol propi...	14338001	21802	40	AR-16-FG-008581-01
Caelo	Clobetasol propi...	14338001	21896	40	1607072

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Clobetasol propi...	1606022	22714	40	20160713*
Caelo	Clobetasol propi...	15439504	22724	40	20160204
Caelo	Clobetasol propi...	14338001	21802SI	39	AR-16-FG-008581-01
Caelo	Clobetasol propi...	14338001	21896SI	30	1607072
Euro OTC	Clobetasol propi...	1606022	22714SI	40	20160713*
Caelo	Clobetasol propi...	15439504	22724SI	37	20160204

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 466 spectra of 11 reference samples from the substance/substance group *Clobetasol propionate*. These samples are listed above in the [calibration samples](#) section.
- 74 030 spectra from a total of 1617 batches from further 372 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 [†].

- 404 spectra of 14 reference samples from the substance/substance group *Clobetasol propionate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clobetasol propionate	13269505	21473 [†]	20
Euro OTC	Clobetasol propionate	1211021-04	21611 [†]	20
Caelo	Clobetasol propionate	14338001	21802 [†]	20
Caelo	Clobetasol propionate	14338001	21896 [†]	19
Caelo	Clobetasol propionate	161067	22470	60
Euro OTC	Clobetasol propionate	1704020	23397	40
Caelo	Clobetasol propionate	170967	23665	40
Euro OTC	Clobetasol propionate	1804002	24075	40
Caelo	Clobetasol propionate	14338001	21802SI [†]	20
Caelo	Clobetasol propionate	14338001	21896SI [†]	15
Caelo	Clobetasol propionate	161067	22470SI	48
Euro OTC	Clobetasol propionate	1704020	23397SI	20
Caelo	Clobetasol propionate	170967	23665SI	20
Euro OTC	Clobetasol propionate	1804002	24075SI	22

*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.

- 126 488 spectra from a total of 2782 batches from further 781 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.

- 1261 spectra from 401 *Apo-Ident* customers from 274 batches from the substance/substance group *Clobetasol propionate*.

Supplier	Substance	Batch	Spectra
Euro OTC	Clobetasol propionate	1108044-01	4
Euro OTC	Clobetasol propionate	1108044-02	6
Caelo	Clobetasol propionate	11101315	1
Fagron	Clobetasol propionate	11300703	1
Caelo	Clobetasol propionate	11300703	4
Euro OTC	Clobetasol propionate	1108044-03	14
Fagron	Clobetasol propionate	12E08-N04	11
Caelo	Clobetasol propionate	1108044-03	2
Caelo	Clobetasol propionate	11300702	3
Caelo	Clobetasol propionate	12107601	3
Euro OTC	Clobetasol propionate	1108044-037-16	1
Caelo	Clobetasol propionate	12107607	6
Euro OTC	Clobetasol propionate	110804404	2
Caelo	Clobetasol propionate	23111202	1
Gehe	Clobetasol propionate	10D21-N04	1
Fagron	Clobetasol propionate	11-05-N06	1
Euro OTC	Clobetasol propionate	1108044-04	14
Fagron	Clobetasol propionate	11L12-N05	1
Caelo	Clobetasol propionate	20121012-4	1
Anzag	Clobetasol propionate	12E08-N04	1
Sanacorp	Clobetasol propionate	1108044-03	1
Caelo	Clobetasol propionate	12107602	3
Caelo	Clobetasol propionate	12107604	1
Audor Pharma	Clobetasol propionate	sieheBemerkung	1
Caelo	Clobetasol propionate	12107608	1
Sanacorp	Clobetasol propionate	12107608	1
Gehe	Clobetasol propionate	12107606	1
Caelo	Clobetasol propionate	11300707	2
Fagron	Clobetasol propionate	12J25-N01	3
Caelo	Clobetasol propionate	12107609	5
Caelo	Clobetasol propionate	3012Q02835	1
Fagron	Clobetasol propionate	11/29-N07	1
Sanacorp	Clobetasol propionate	12107609	2
Fagron	Clobetasol propionate	11D26-N04	1
Caelo	Clobetasol propionate	12342303	1
Fagron	Clobetasol propionate	NS0486M	1
Euro OTC	Clobetasol propionate	1108044	1
Fagron	Clobetasol propionate	NS0292-M	1
Euro OTC	Clobetasol propionate	1211021-01	18

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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
Symbiotica Spec./Phönix	Clobetasol propionate	CL0-B12153/0711	1
Caelo	Clobetasol propionate	1108044-04	1
Euro OTC	Clobetasol propionate	2111I-02835	1
Alliance Healthcare	Clobetasol propionate	12J25-N01	1
Noweda	Clobetasol propionate	11300702	1
Caelo	Clobetasol propionate	12342306	6
Euro OTC	Clobetasol propionate	1105044-04	1
Sanacorp	Clobetasol propionate	1211021-01	1
Caesar/Lorenz	Clobetasol propionate	12342305	3
Caelo	Clobetasol propionate	1108044-02	1
Euro OTC	Clobetasol propionate	121102101	2
Fagron	Clobetasol propionate	13A02-N04	16
Noweda	Clobetasol propionate	12342305	1
Gehe	Clobetasol propionate	12342306	2
Phönix Gotha	Clobetasol propionate	1108044-04	1
	Clobetasol propionate	11/29-N07	1
Phönix	Clobetasol propionate		1
Bombastus	Clobetasol propionate	12342303	1
Caelo	Clobetasol propionate	12342309	12
Euro OTC	Clobetasol propionate	121K021-01	1
euroho/gehe	Clobetasol propionate	1211021-01	1
Euro OTC	Clobetasol propionate	CL0-BL2322/1012	2
Caelo	Clobetasol propionate	12342307	2
Caelo	Clobetasol propionate	31071302	1
Caelo	Clobetasol propionate	12J25-N01	1
Euro OTC	Clobetasol propionate	1211021-02	27
Caesar & Loretz/ Noweda	Clobetasol propionate	12342306	1
Euro OTC	Clobetasol propionate	12082013B	1
Gehe	Clobetasol propionate	12342310	1
Fagron	Clobetasol propionate	13G23N01	1
Caelo	Clobetasol propionate	13A02-N04	1
Fagron	Clobetasol propionate	13G23-N01	16
Fagron	Clobetasol propionate	3713M-02835	1
Euro OTC	Clobetasol propionate	12110-01	1
Caelo	Clobetasol propionate	12342310	7
Caesar u Loretz	Clobetasol propionate	12107608	2
Caelo	Clobetasol propionate	13134703	4
Euro	Clobetasol propionate	1211021-02	2
Fagron	Clobetasol propionate	12E08N04	1
Phönix Gotha	Clobetasol propionate	1211021-02	3
Caelo	Clobetasol propionate	13134702	7
Caesar/Loretz	Clobetasol propionate	12342310	1
Fagron	Clobetasol propionate	13G23-N01	1
Fagron	Clobetasol propionate	13A02-N04	1
Sanacorp	Clobetasol propionate	12342310	1
Phoenix 29.11.12	Clobetasol propionate	700225	2
Noweda	Clobetasol propionate	12342310	1
Caelo	Clobetasol propionate	12342312	1
Caesar/Lorenz	Clobetasol propionate	12342309	1
Caelo	Clobetasol propionate	13134701	14
Euro OTC	Clobetasol propionate	1211021-03	26
Anzag	Clobetasol propionate	1211021-02	1
Fagron	Clobetasol propionate	1211021-02	1
symbiotica/gehe	Clobetasol propionate	1211021-03	1
Symbiotica Spec.	Clobetasol propionate	1211021-03	1
Caelo	Clobetasol propionate	13134704	4
Fagron	Clobetasol propionate	13G23-N01NT0421M	1
Alliance Health 17.01.2...	Clobetasol propionate	APB00547/112010C	1
Caelo	Clobetasol propionate	13G23-N01	1
Caelo	Clobetasol propionate	15031401	1

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Supplier	Substance	Batch	Spectra
Caelo	Clobetasol propionate	13134705	4
Caelo	Clobetasol propionate	13269501	1
GEHE 21.03.2014	Clobetasol propionate	1211021-02	1
Fagron	Clobetasol propionate	1314705	1
Noweda	Clobetasol propionate	13134701	1
Phoenix 02.04.2014	Clobetasol propionate	1211021-03	3
Fagron	Clobetasol propionate	11129-N07	1
Noweda/Anzag	Clobetasol propionate	13269504	3
Euro OTC	Clobetasol propionate	16042014C	1
Noweda	Clobetasol propionate	13134705	1
Crystal Pharma	Clobetasol propionate	C0054/1	1
Caelo	Clobetasol propionate	13269502	3
Fagron	Clobetasol propionate	1211021	1
Fagron	Clobetasol propionate	NT0421M	3
Caelo	Clobetasol propionate	13K08-B30-287728	1
Chiesi/ Now	Clobetasol propionate	13269503	3
Caelo	Clobetasol propionate	13269504	5
Euro OTC	Clobetasol propionate	130604002	1
Raben-Apotheke Mildenau	Clobetasol propionate	13k08-b30-287727	1
Fagron	Clobetasol propionate	13K08-B30-287728	5
Euro OTC	Clobetasol propionate	1211021-04	19
Caelo	Clobetasol propionate	13269508	11
Symbiotica Spec./Phönix	Clobetasol propionate	1108044-04	1
Fagron	Clobetasol propionate	13K08-B30-287730	2
Caelo	Clobetasol propionate	13K08-B30-287726	1
Phoenix	Clobetasol propionate	13K08B30287728	1
Euro OTC	Clobetasol propionate	30092014A	1
Sanacorp	Clobetasol propionate	13g23n01	1
Bombastus	Clobetasol propionate	13G23-N0	1
Bombastus	Clobetasol propionate	13G23-N01	1
sanacorp	Clobetasol propionate	13269508	1
Caelo	Clobetasol propionate	2014E-02835	1
Caelo	Clobetasol propionate	14188502	6
Phönix Caesar u. Loretz	Clobetasol propionate	13269508	1
Caelo	Clobetasol propionate	13269509	1
Fagron	Clobetasol propionate	13k08b30287728	1
Fagron	Clobetasol propionate	13K08-B30	2
Euro OTC	Clobetasol propionate	1211021/02	1
Caelo	Clobetasol propionate	14102416	1
Caelo	Clobetasol propionate	14188504	6
Fagron	Clobetasol propionate	13K08B30287730	1
Fagron	Clobetasol propionate	13K08-B30-287729	2
EuRho	Clobetasol propionate	1408018-01	1
Audor Pharma	Clobetasol propionate	APB0054/112010C	1
Caelo	Clobetasol propionate	1369504	1
Fagron	Clobetasol propionate	13K08-B30-287726	2
Fagron	Clobetasol propionate	14C03-B07-293562	9
Caelo	Clobetasol propionate	14188501	3
Gehe	Clobetasol propionate	14188504	1
Euro OTC	Clobetasol propionate	1408018-01	12
Fagron	Clobetasol propionate	14C03-B07	2
Caelo	Clobetasol propionate	14188503	14
Caelo	Clobetasol propionate	13269507	3
Fagron	Clobetasol propionate	13K08-B30-287727	1
Euro OTC	Clobetasol propionate	1408015-01	1
Sanacorp;19.03.15;87,60EUR	Clobetasol propionate	14C03-B07-293563	1
Sanacorp	Clobetasol propionate	13269507	1
Euro OTC	Clobetasol propionate	13042015A	1
Fagron	Clobetasol propionate	14G30-B07-302115	2
Fagron	Clobetasol propionate	14C03-B07-293561	2

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Supplier	Substance	Batch	Spectra
Fagron	Clobetasol propionate	13K08-B03-287728	1
Anzag	Clobetasol propionate	1408018-01	2
Fagron	Clobetasol propionate	14C03-B07-293563	1
Caelo	Clobetasol propionate	14C03-B07-293560	2
Caelo	Clobetasol propionate	14338002	1
Euro OTC	Clobetasol propionate	1408018-02	61
Fargon	Clobetasol propionate	14C03-B07	1
Caelo	Clobetasol propionate	14338001	9
Caelo	Clobetasol propionate	11101311	1
Allianz Healthcare 02.0...	Clobetasol propionate	1408018-01	1
Fagron	Clobetasol propionate	14188502	1
Euro OTC	Clobetasol propionate	1072015D	1
Caelo	Clobetasol propionate	14338005	3
Fagron	Clobetasol propionate	14G30-B07-303114	1
Fagron	Clobetasol propionate	14C03-B07-293560	1
Fagron	Clobetasol propionate	11C16-N01	1
Caelo	Clobetasol propionate	apl/294/b-14	1
Fagron	Clobetasol propionate	14G30-B07-302116	4
Euro OTC	Clobetasol propionate	700225	1
Caelo	Clobetasol propionate	1408018-02	10
Caelo	Clobetasol propionate	1438007	1
Caelo	Clobetasol propionate	14g30bo7302114	1
Fagron	Clobetasol propionate	14G30-B07-302114	10
Caelo	Clobetasol propionate	14188506	3
Caelo	Clobetasol propionate	14G30-B07-302114	2
Euro OTC	Clobetasol propionate	140801801	1
Euro OTC	Clobetasol propionate	4091512	1
Fischar	Clobetasol propionate	14188506	1
Audor Pharma	Clobetasol propionate	APL/035/E-12C	1
Caelo	Clobetasol propionate	14338006	11
Caelo	Clobetasol propionate	14338008	4
Fagron	Clobetasol propionate	15A14-B02-303125	10
Hedinger/ Sanacorp	Clobetasol propionate	APAPL/035/E-12C	1
Anzag	Clobetasol propionate	15246001	1
Farmabios S.p.A./Caesar...	Clobetasol propionate	14338006	1
Fagron	Clobetasol propionate	14G30-B07-302113	2
Audor Pharma	Clobetasol propionate	APAPL/035/E-12C	2
Caelo	Clobetasol propionate	15A14-B02	1
Caelo	Clobetasol propionate	15246001	6
Caelo	Clobetasol propionate	15234003	16
Caelo	Clobetasol propionate	14338007	5
Euro OTC	Clobetasol propionate	140808-02	1
Gehe	Clobetasol propionate	15234003	1
Caelo	Clobetasol propionate	14G30B07302114	1
Sanacorp	Clobetasol propionate	15234003	1
Fagron	Clobetasol propionate	14G30B07302112	1
Euro OT	Clobetasol propionate	14081018-02	1
Fagron	Clobetasol propionate	15C23-B02-310473	10
Fagron	Clobetasol propionate	15a14-b02-303125	2
Fagron	Clobetasol propionate	14C03-B07-305987	2
Caelo	Clobetasol propionate	15234004	20
Fagron	Clobetasol propionate	14G30-B07-302112	2
Caelo	Clobetasol propionate	1524003	1
Caelo	Clobetasol propionate	15C23-B02-310473	1
WE: 20.01.16	Clobetasol propionate	15234004	1
Caelo	Clobetasol propionate	15234001	7
sanacorp	Clobetasol propionate	14188506	1
Caelo	Clobetasol propionate	15234002	1
Caelo	Clobetasol propionate	152340004	1
Caesar&Loretz GmbH	Clobetasol propionate	15234001	1

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Supplier	Substance	Batch	Spectra
Noweda	Clobetasol propionate	14338007	1
Fagron	Clobetasol propionate	15H26-B03-312860	1
Fagron	Clobetasol propionate	15C23-B02-310522	2
Caelo	Clobetasol propionate	15234009	4
Alliance H.	Clobetasol propionate	15234002	2
Fagron	Clobetasol propionate	1405018-02	1
HCK	Clobetasol propionate	11/05-N06	1
Caelo	Clobetasol propionate	15439503	18
Fgaron	Clobetasol propionate	15H26-B03	1
allianz	Clobetasol propionate	15234009	1
Caelo	Clobetasol propionate	123645	1
Noweda	Clobetasol propionate	15234004	1
Caelo	Clobetasol propionate	1408018-03	9
Fagron	Clobetasol propionate	15c23-b02-310473	2
Euro OTC	Clobetasol propionate	15234003	1
Euro OTC	Clobetasol propionate	1408018-03	22
Audor Pharma	Clobetasol propionate	APL035E12C	1
Euro OTC	Clobetasol propionate	80616-1	1
Fagron	Clobetasol propionate	15H26-B03-312355	2
Caelo	Clobetasol propionate	15439501	4
Fagron	Clobetasol propionate	15J15-B04-316615	1
Caelo	Clobetasol propionate	15439502	6
Fagron	Clobetasol propionate	15J15-B04-317698	5
phönix	Clobetasol propionate	15439503	1
Caelo	Clobetasol propionate	15439504	20
phönix	Clobetasol propionate	15439504	1
Fagron	Clobetasol propionate	15C23-B02310473	2
Caesar&Loretz GmbH	Clobetasol propionate	15439501	1
Fagron	Clobetasol propionate	16E04-B12-321034	2
Fagron	Clobetasol propionate	16E04-B12-321036	1
Caelo	Clobetasol propionate	15J-15-B04-316616	1
Cacolo/Noweda	Clobetasol propionate	15439503	1
Caelo	Clobetasol propionate	15234008	1
Caelo	Clobetasol propionate	160829CP	1
Caelo	Clobetasol propionate	160115CP	1
Symbiotica/Sanacorp	Clobetasol propionate	1408018-03	1
Caelo	Clobetasol propionate	16E04-B12-321036	1
Caelo	Clobetasol propionate	16106702	10
Caelo	Clobetasol propionate	16106703	11
Noweda/ Ichthyol	Clobetasol propionate	15439503	1
Fagron	Clobetasol propionate	16E04-B12-322020	4
Euro OTC	Clobetasol propionate	1606022-01	15
Caelo	Clobetasol propionate	15j15-b04-317698	1
Caelo	Clobetasol propionate	1606022-01	3
Caelo	Clobetasol propionate	15253032	1
Caelo	Clobetasol propionate	160602201	1
Euro OTC	Clobetasol propionate	160602201	4
Caelo	Clobetasol propionate	15439507	2
Caelo	Clobetasol propionate	16E04-B12	1
Phoenix	Clobetasol propionate	15439502	1
Symbiotica/Noweda	Clobetasol propionate	1606022-01	1
Caelo	Clobetasol propionate	154390504	1
20.12.2016 Phoenix 17,49EUR	Clobetasol propionate	15439504	1
Euro OTC	Clobetasol propionate	1601046-01	1
Caelo	Clobetasol propionate	CL0024/0915	1
Caelo	Clobetasol propionate	1616703	1
Caelo	Clobetasol propionate	16106704	14
Euro OTC	Clobetasol propionate	140801803	1
Phönix	Clobetasol propionate	16106703	1
Caelo	Clobetasol propionate	18H22-B017-328012	1

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Supplier	Substance	Batch	Spectra
Caelo	Clobetasol propionate	16H22-B07-328012	1
Fagron	Clobetasol propionate	16E04-B12	1
Fagron	Clobetasol propionate	15J15-B04	1
PhönixWE24.10.2014 EK...	Clobetasol propionate	1211021-04	1
Gehe	Clobetasol propionate	1606022-01	1
Fagron	Clobetasol propionate	16E04-B12-321033	2
Fagron	Clobetasol propionate	15j15-B04-317698	1
Euro OTC	Clobetasol propionate	1606022-02	24
Fagron	Clobetasol propionate	16G18-B02-325573	5
Fagron	Clobetasol propionate	16E04-B12-321032	1
Caelo	Clobetasol propionate	12E08-N04	1
Euro OTC	Clobetasol propionate	160602202	3
Euro OTC	Clobetasol propionate	4113Q-02835	1
Phoenix	Clobetasol propionate	16h22-b07-328012	1
Caelo	Clobetasol propionate	16106709	9
Sanacorp	Clobetasol propionate	1606022-02	2
Fagron	Clobetasol propionate	16G18-B02-325571	2
Fagron	Clobetasol propionate	16G18-B02-324627	4
Caelo	Clobetasol propionate	16106701	2
Noweda/EuRo	Clobetasol propionate	1606022-01	1
Audor Pharma	Clobetasol propionate	APCLP/M/036/16C	1
Fagron	Clobetasol propionate	15/15-B04-317699	1
Noweda/Apomix	Clobetasol propionate	16106703	1
Caelo	Clobetasol propionate	181016709	1
Gehe	Clobetasol propionate	16106704	1
Caelo	Clobetasol propionate	170404CP1606022-02	1
Noweda 6.4.17	Clobetasol propionate	1606022-01	1
Phoenix WE 29.04.17 -15...	Clobetasol propionate	1606022-02	1
Fagron	Clobetasol propionate	16H22-B07-328012	11
Caelo	Clobetasol propionate	16106713	6
EuRho/Phoenix	Clobetasol propionate	160602202	1
Gehe	Clobetasol propionate	16106701	1
Fagron	Clobetasol propionate	16G18-B02-32571	1
Caelo	Clobetasol propionate	16106715	5
Caelo	Clobetasol propionate	16106711	13
Caesar&Lorenz	Clobetasol propionate	1610370	1
phönix	Clobetasol propionate	16106704	1
Fagron	Clobetasol propionate	16H22-B07-330169	3
Caelo	Clobetasol propionate	16106710	3
Fagron	Clobetasol propionate	16H22-B07	1
Euro OTC	Clobetasol propionate	1606022	2
Caelo	Clobetasol propionate	1606022-02	2
Noweda	Clobetasol propionate	16106720	1
Finteler Apotheke	Clobetasol propionate	16K24-B04-333121	2
Fagron	Clobetasol propionate	1606022-02	1
Fagron	Clobetasol propionate	16K24-B04-332086	5
Caelo	Clobetasol propionate	16106712	3
Caelo	Clobetasol propionate	1606022-025349	1
Fagron	Clobetasol propionate	16G18-B02-325572	1
Euro OTC	Clobetasol propionate	1704020-01	40
Caelo	Clobetasol propionate	17096702	5
Noweda	Clobetasol propionate	1606022-02	1
GEHE	Clobetasol propionate	16G18-B02-324627	1
Caelo	Clobetasol propionate	16106720	3
Euro OTC	Clobetasol propionate	170402001	2
Euro OTC	Clobetasol propionate	171107CP/1704020-01	1
Fagron	Clobetasol propionate	16K24-B04-333120	1
Phönix	Clobetasol propionate	17096706	1
Euro OTC	Clobetasol propionate	c1o-bl1t223/126	1
Caeolo/Krieger	Clobetasol propionate	17096706	3

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Supplier	Substance	Batch	Spectra
Caelo	Clobetasol propionate	16C18-B02-325573	1
Fagron	Clobetasol propionate	16K24-B04-333120	1
Caelo	Clobetasol propionate	17096706	5
Fagron	Clobetasol propionate	17E04-B02-338441	1
Gehe	Clobetasol propionate	17096705	1
Noweda	Clobetasol propionate	17096706	1
Caelo	Clobetasol propionate	17096705	7
Caelo	Clobetasol propionate	17096701	6
gehe	Clobetasol propionate	APCLPM03616C	1
Caelo	Clobetasol propionate	170402001	1
Fagron	Clobetasol propionate	16K24-B04-333143	1
Phoenix/Cealo	Clobetasol propionate	17096701	1
Fagron	Clobetasol propionate	17G14-B12-340176	2
Caelo	Clobetasol propionate	17096704	1
Caelo	Clobetasol propionate	16106718	1
Euro OTC	Clobetasol propionate	1704020-015498	1
Gehe	Clobetasol propionate	17096708	1
Caelo	Clobetasol propionate	17096708	8
Fagron	Clobetasol propionate	17G14-B12-340175	3
Caelo	Clobetasol propionate	1704020-01	10
Caelo	Clobetasol propionate	17096709	3
Delta	Clobetasol propionate	17096701	1
Caelo	Clobetasol propionate	16353208	1
Fagron	Clobetasol propionate	17E04-B02-336882	1
Caelo	Clobetasol propionate	17325603	9
Caelo	Clobetasol propionate	17325602	9
euro AHD	Clobetasol propionate	1704020-015592	1
Caelo	Clobetasol propionate	1735603	1
Caelo	Clobetasol propionate	17096707	2
Caelo	Clobetasol propionate		1
Caelo	Clobetasol propionate	1704020	1
Caelo	Clobetasol propionate	17090708	1
Anzag	Clobetasol propionate	16106703	1
Caeolo	Clobetasol propionate	17096709	1
Symbiotica / Noweda	Clobetasol propionate	1704020-01	1
Fagron	Clobetasol propionate	17G14-B12-341742	1
Caelo	Clobetasol propionate	17325606	1
EuRho/Gehe	Clobetasol propionate	1704020-01	1
Euro OTC	Clobetasol propionate	1804002-01	13
Fagron	Clobetasol propionate	17G14-B12-341743	1
Jenne	Clobetasol propionate	17325601	2
Caelo	Clobetasol propionate	2x17325602	1
Caelo	Clobetasol propionate	18082703	6
Caelo	Clobetasol propionate	1105044-03	1
Caelo	Clobetasol propionate	17325601	4
Caelo	Clobetasol propionate	17E04-B02-336882	1
Caelo	Clobetasol propionate	17L18-B02-347993	1
Fagron	Clobetasol propionate	17L18-B02-344842	2
Allianz	Clobetasol propionate	17325606	1
Fagron	Clobetasol propionate	17L18-B02-345404	2
Caelo	Clobetasol propionate	17G14-B12-341742	1
Caelo	Clobetasol propionate	18082702	1
Caelo	Clobetasol propionate	17325605	4
euro AHD	Clobetasol propionate	1804002-015788	1
Euro OTC	Clobetasol propionate	18082703	1
Fagron	Clobetasol propionate	17L18-B02-347993	1
Caelo	Clobetasol propionate	18082708	2
Caelo	Clobetasol propionate	18082710	1

- 77 668 spectra from 564 *Apo-Ident* customers from a total of 25 870 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	466	0	74 030
Type B	0	404	0	126 488
Type C	0	1245	16	77 668

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.7124 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.5149 %)
Type C	100.0000 % (> 99.8817 %)	98.7312 % (> 98.4933 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21092	21092	0.00	18.21
21611	21611	0.00	18.10
21802	21802	0.00	30.08
22714	22714	0.00	15.67
22724	21092	4.04	16.41
21473	21473	0.00	22.96
21896	21896	0.00	19.08

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Clonidine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20637-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Clonidine hydrochloride; Clonidini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Clonidine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Clonidine hydroc...	13I25-B07	21220	40	20131009
Fagron	Clonidine hydroc...	14H11-B04-311163	21966	40	AR-18-FG-006797-02
Fagron	Clonidine hydroc...	14H11-B04-311163	22967	40	20140929
Fagron	Clonidine hydroc...	14H11-B04-311163	22967SI	40	20140929

Validation samples

A total of 280 317 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 *Clonidine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1621 batches from further 372 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 8 reference samples from the substance/substance group *Clonidine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Clonidine hydrochloride	14H11-B04-311163	21966 [†]	20
Fagron	Clonidine hydrochloride	15L11-B01-332270	23228	40
Fagron	Clonidine hydrochloride	15L11-B01-332270	23410	40
Fagron	Clonidine hydrochloride	18B12-B04-353341	24443	40
Fagron	Clonidine hydrochloride	14H11-B04-311163	21966SI	60
Fagron	Clonidine hydrochloride	15L11-B01-332270	23228SI	40
Fagron	Clonidine hydrochloride	15L11-B01-332270	23410SI	40
Fagron	Clonidine hydrochloride	18B12-B04-353341	24443SI	40

- 126 572 spectra from a total of 2786 batches from further 781 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*.

- 43 spectra from 5 *Apo-Ident* customers from 2 batches from the substance/substance group *Clonidine hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	Clonidine hydrochloride	14H11-B04-311163	42
Fagron	Clonidine hydrochloride	14H11-B04-298642	1

- 78 886 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Clonidine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clonidine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	317	3	126 572
Type C	0	43	0	78 886

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	99.0625 % (> 98.1250 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 86.0465 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21220	21966	10.74	55.32
21966	21966	0.00	71.73
22967	21966	12.43	52.39

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Clotrimazole**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20000-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Clotrimazole; Clotrimazolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Clotrimazole	12I21-N01	20794	40	20120322
Caelo	Clotrimazole	13184113	21087	40	20130614
Caelo	Clotrimazole	13224204	21114	40	20130815
Euro OTC	Clotrimazole	1306036-01	21207	40	20130823
Fagron	Clotrimazole	14B05-B36	21259	40	20140225

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Clotrimazole	14C04-B31	21264	40	20140319
Caelo	Clotrimazole	13224220	21352	40	20130815
Euro OTC	Clotrimazole	1510003	22229	40	20151111*
Caelo	Clotrimazole	153956	23791	40	20151215*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Clotrimazole*. These samples are listed above in the [calibration samples](#) section.
- 74 136 spectra from a total of 1614 batches from further 372 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 [†].

- 290 spectra of 8 reference samples from the substance/substance group *Clotrimazole*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clotrimazole	12320815	20861	30
Caelo	Clotrimazole	13224220	21353	40
Euro OTC	Clotrimazole	1510003	22229 [†]	20
Euro OTC	Clotrimazole	1607046	22793	40
Euro OTC	Clotrimazole	1703028	23129	40
Caelo	Clotrimazole	171116	23322	40
Caelo	Clotrimazole	17111616	23781	40
Euro OTC	Clotrimazole	1808028	24298	40

- 126 602 spectra from a total of 2781 batches from further 781 substances. These spectra were

*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*.

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.

- 1836 spectra from 449 *Apo-Ident* customers from 394 batches from the substance/substance group *Clotrimazole*.

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	11E17-N10	1
Fagron	Clotrimazole	11A05-N14	2
Caelo	Clotrimazole		6
Caelo	Clotrimazole	11-K21-N19	1
Caelo	Clotrimazole	10247328	3
Fagron	Clotrimazole	11K21-N19	1
Caelo	Clotrimazole	1105014-02	1
Euro OTC	Clotrimazole	1108053-01	1
Caelo	Clotrimazole	11/22-N10	1
Euro OTC	Clotrimazole	1105014-02	1
Fagron	Clotrimazole	12A05-N10	2
Fagron	Clotrimazole	12E02-N12	8
Fagron	Clotrimazole	11L12-N10	4
Caelo	Clotrimazole	11305506	2
Euro OTC	Clotrimazole	1203040-01	1
Gehe	Clotrimazole	1108053-01	1
Euro OTC	Clotrimazole	700135	2
phönix	Clotrimazole	11305513	1
Euro OTC	Clotrimazole	1209211276	1
Euro OTC	Clotrimazole	1203040	1
Caelo	Clotrimazole	12159902	11
Fagron	Clotrimazole	12a05-n10	1
Phoenix	Clotrimazole	12A05-N10	1
Caelo	Clotrimazole	11305513	7
Fagron	Clotrimazole	20111018	2
Caelo	Clotrimazole	20111115	1
Europharm/Otto	Clotrimazole	1203040-01	1
Caelo	Clotrimazole	12159904	2
Fagron	Clotrimazole	12I21N04	1
Euro OTC	Clotrimazole	1203040-02	8
EuRho	Clotrimazole	1108053-02	1
Sanacorp	Clotrimazole	12159902	1
Fagron	Clotrimazole	12I21-N04	7
Caelo	Clotrimazole	11305511	1
Caelo	Clotrimazole	12159911	2
Fagron	Clotrimazole	20151112-3	1
Fagron	Clotrimazole	12e02-N12	1
Euro OTC	Clotrimazole	1108053-02	1
Euro OTC	Clotrimazole	1203040-03	9
Sanacorp	Clotrimazole	1203040-03	1
Caelo	Clotrimazole	12159916	6
Caelo	Clotrimazole	12E02-N12	2
Noweda	Clotrimazole	1203040-03	2
Fagron	Clotrimazole	12/21-N04	3
Fagron	Clotrimazole	11G15-N10	1
Fagron	Clotrimazole	C22H17CIN2	1

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Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	12121-N04	1
Caelo	Clotrimazole	12159913	9
Fagron	Clotrimazole	12F02-N12	1
Fagron	Clotrimazole	12E30-N07	11
Europharm/Otto	Clotrimazole	1203040-02	1
Euro OTC	Clotrimazole	1105014-01	1
Fagron	Clotrimazole	20120603	3
Caelo	Clotrimazole	12320807	4
Fagron	Clotrimazole	12/21-N01	5
Caelo	Clotrimazole	12320805	3
Fagron	Clotrimazole		2
Fagron	Clotrimazole	1221n04	1
Caelo	Clotrimazole	20111018	1
Caelo	Clotrimazole	700135-0006	1
Euro OTC	Clotrimazole	1210039-01	23
Euro OTC	Clotrimazole	3912E-01276	1
Fagron	Clotrimazole	9041304	1
Noweda	Clotrimazole	20111115	1
Fagron	Clotrimazole	4812E-01276 (NP)	1
Caelo	Clotrimazole	12320809	4
Caelo	Clotrimazole	12320808	11
Caelo	Clotrimazole	1259913	1
Fagron	Clotrimazole	12I21-N01	6
Caelo	Clotrimazole	1234567	1
EUro/AHD	Clotrimazole	1210039-01	2
Fagron	Clotrimazole	13C25-N10	9
Caelo	Clotrimazole	12E30-N07	1
Fagron	Clotrimazole	1221N04	1
Euro OTC	Clotrimazole	2313M01276	1
Caelo	Clotrimazole	12I21-N04	1
Caelo	Clotrimazole	12320806	2
EuRho	Clotrimazole	1203040-02	1
Caelo	Clotrimazole	12B27-N05	2
Fiebig 10.06.13 ek: 8,58EUR	Clotrimazole	12E30-N07	1
Fagron	Clotrimazole	12I16-N04	1
Fagron	Clotrimazole	12K15-N01	1
Caelo	Clotrimazole	12320813	2
Fischar/Gehe	Clotrimazole	20111018	1
Caelo	Clotrimazole	12320814	9
Sanacorp	Clotrimazole	12320814	1
Caelo	Clotrimazole	13148007	1
Caelo	Clotrimazole	13184103	8
Caelo	Clotrimazole	26071305	1
Euro OTC	Clotrimazole	110501402	1
Caelo	Clotrimazole	1882321	1
Fagron	Clotrimazole	12B27-N05	2
Gehe	Clotrimazole	12/21-N01	1
Caesar/Lorenz	Clotrimazole	12320814	1
Sanacorp	Clotrimazole	1230805	1
Euro OTC	Clotrimazole	12082013C	1
Caelo	Clotrimazole	12320815	1
Fagron	Clotrimazole	1210039-01	1
Euro OTC	Clotrimazole	121003901	2
Phönix	Clotrimazole	13C25-N10	1
Sanacorp	Clotrimazole	13184105	1
Caelo	Clotrimazole	1210039-01	1
Caelo	Clotrimazole	13184105	12
Euro OTC	Clotrimazole	1210039-02	18
AHD	Clotrimazole	13184105	1
Gehe	Clotrimazole	11K21-N19	1

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Supplier	Substance	Batch	Spectra
Europ Ots Pharma	Clotrimazole	13184105	1
Caelo	Clotrimazole	11305507	1
Caelo	Clotrimazole	13184111	6
Caelo	Clotrimazole	13224201	21
Caesar&Loretz GmbH/Anzag	Clotrimazole	13184111	1
Caelo	Clotrimazole	13184113	2
Caelo	Clotrimazole	311111	1
Caelo	Clotrimazole	1210030-02	1
Caelo	Clotrimazole	131841111	1
Bombastus	Clotrimazole	12320815	1
Euro OTC	Clotrimazole	1306036-01	36
EuRho	Clotrimazole	1306036-01	2
Euro OTC	Clotrimazole	120304002	1
Euro OTC	Clotrimazole	21122013A	1
Caelo	Clotrimazole	1306036-01	3
Gehe	Clotrimazole	1306036-01	2
Caesar/Lorenz	Clotrimazole	13224201	3
Caelo	Clotrimazole	13224210	10
Caelo	Clotrimazole	PC85	1
Sino Phyto	Clotrimazole	13224210	2
Caelo	Clotrimazole	1322401	1
Caelo	Clotrimazole	13224211	5
Noweda	Clotrimazole	13224201	1
Caelo	Clotrimazole	11081201	1
PHOENIX am 22.01.2014	Clotrimazole	1306036-01	1
Caelo	Clotrimazole	13224212	8
Euro OTC	Clotrimazole	1306306-01	1
Fagron	Clotrimazole	13224201	1
Euro OTC	Clotrimazole	130636-01	2
EuRho/Phönix	Clotrimazole	1210039-2	1
Euro OTC	Clotrimazole	130603601	3
Caelo	Clotrimazole	412091-2-P	1
europharma	Clotrimazole	1306036-01	1
EuRho	Clotrimazole	1210039-02	2
Sanacorp	Clotrimazole	13224214	2
Caelo	Clotrimazole	13224214	8
Caelo	Clotrimazole	13224216	9
Euro OTC	Clotrimazole	1314Q1276	1
Caelo	Clotrimazole	13224204	2
Caelo	Clotrimazole	1309034-C1	1
Gehe	Clotrimazole	13224216	1
Caelo	Clotrimazole	156546	1
Euro OTC	Clotrimazole	15042014C	1
Fagron	Clotrimazole	14B05-B36	7
Caelo	Clotrimazole	132234216	1
EuRho/Phoenix	Clotrimazole	1210039-02	1
Caelo	Clotrimazole	13224220	6
Caelo	Clotrimazole	13224217	7
Caelo	Clotrimazole	415050-2-P	1
Euro OTC	Clotrimazole	1309034-01	18
Fagron	Clotrimazole	14C04B32291657	1
Fagron	Clotrimazole	14B05-B36-291168	2
Caelo	Clotrimazole	13324204	1
	Clotrimazole	14C04-B30-291661	1
Sanacorp	Clotrimazole	105/AKD1	1
Fagron	Clotrimazole	14C04-B30-291656	9
Noweda	Clotrimazole	13224217	1
Fagron	Clotrimazole	1309034-01	3
Caelo	Clotrimazole	1306036	1
Euro OTC	Clotrimazole	1309034-02	18

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Supplier	Substance	Batch	Spectra
Caelo	Clotrimazole	13224215	3
Euro OTC	Clotrimazole	20130512	1
Caelo	Clotrimazole	160614	1
	Clotrimazole	1306036-01	1
Euro OTC	Clotrimazole	15072014A	1
Vdl 14.07.14	Clotrimazole	13224225	1
Fagron	Clotrimazole	14B05-B36-291166	3
Caelo	Clotrimazole	13224218	11
Fagron	Clotrimazole	14B05-B36-291167	5
Euro OTC	Clotrimazole	130903401	4
Alliance Healthcare	Clotrimazole	1309034-01	1
Phoenix	Clotrimazole	13224215	1
Apomix	Clotrimazole	14B05-B36	1
Fagron	Clotrimazole	CLT/1307/0065A	2
Caelo	Clotrimazole	13224225	2
Caelo	Clotrimazole	13224221	2
Caelo	Clotrimazole	418072-1-P	1
EuRho	Clotrimazole	1309034-02	1
Caelo	Clotrimazole	14c04-b30-291656	1
Audor Pharma	Clotrimazole	AP1306036-01C	1
Caelo	Clotrimazole	13224219	6
Euro OTC	Clotrimazole	2214A-01276	1
Caelo	Clotrimazole	14144905	17
Caelo	Clotrimazole	130603601	1
Euro OTC	Clotrimazole	1306036	1
Sanacorp	Clotrimazole	14144905	1
Euro OTC	Clotrimazole	1309034	1
Caelo	Clotrimazole	1309034-02	2
Fagron	Clotrimazole	14b05-B36-291167	1
Fagron	Clotrimazole	14b05b36291166	1
Fagron	Clotrimazole	14223201	1
Fagron	Clotrimazole	14C04-B31-294939	6
Fagron	Clotrimazole	14B05-B35-293543	1
Fagron	Clotrimazole	14B05-B35-293544	5
Caelo	Clotrimazole	14144912	2
Caelo	Clotrimazole	14144911	12
Fagron	Clotrimazole	14C04-B31-291660	1
Fagron	Clotrimazole	14C04-B31	6
eurho	Clotrimazole	1309034-02	2
Euro OTC	Clotrimazole		2
Fagron	Clotrimazole	14B05-B35-293542	3
Euro OTC	Clotrimazole	1409027-01	25
Fagron	Clotrimazole	14b05-b36-291166	1
Gehe	Clotrimazole	1309034-01	1
Fagron	Clotrimazole	14B05-B35	2
Euro OTC	Clotrimazole	22122014B	1
Caelo	Clotrimazole	14C04-B30-291656	2
Caelo	Clotrimazole	Fagron	1
Euro OTC	Clotrimazole	14C04-B31-291660	1
Phoenix 23.10.14 5,50	Clotrimazole	1309034-02	1
Fagron	Clotrimazole	14C04-B30-291661	2
Euro OTC	Clotrimazole	1309054-02	1
Caesar&loretz,Phoenix	Clotrimazole	14144912	1
Caelo	Clotrimazole	14144918	11
Phoenix	Clotrimazole	1309034-02	1
Sanacorp	Clotrimazole	13224219	1
Euro OTC	Clotrimazole	140927-01	1
Caelo	Clotrimazole	14144917	5
Euro OTC	Clotrimazole	1409027	6
Caelo	Clotrimazole	14337801	11

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Supplier	Substance	Batch	Spectra
Caelo	Clotrimazole	14144913	2
EuRho/Phoenix	Clotrimazole	1409027-01	1
Fagron	Clotrimazole	14B05-B36-291165	2
EuRho	Clotrimazole	1409027-01	1
Caelo	Clotrimazole	14337802	7
Gehe	Clotrimazole	14C04-B31-294952	1
A.H.D.	Clotrimazole	14337801	1
Fagron	Clotrimazole	14B05-B36-2991166	1
Fagron	Clotrimazole	14337801	1
Euro OTC	Clotrimazole	1409027-02	33
Fagron	Clotrimazole	14B05B36291167	1
Caelo	Clotrimazole	14144914	8
Fagron	Clotrimazole	14C04-B31-294951	1
Caelo	Clotrimazole	14C04-B31-294939	1
Anzag	Clotrimazole	14C04-B30-2916618	1
sanacorp	Clotrimazole	14144918	1
Euro OTC	Clotrimazole	14144914	1
Euroo / Phönix	Clotrimazole	1409027-02	3
Euro OTC	Clotrimazole	21052015B	1
Fagron	Clotrimazole	14B05-B35-294932	1
Fagron	Clotrimazole	14C04-B31-299954	4
Caelo	Clotrimazole	1409027-02	2
Caelo	Clotrimazole	14337807	9
Fagron	Clotrimazole	14b05-b35-293544	1
Fagron	Clotrimazole	14B05-B35-294935	4
VDL;11.06.15;27,90EUR	Clotrimazole	14337807	1
Fagron	Clotrimazole	14C04-B31-294940	1
Fagron	Clotrimazole	14C04-B31-294952	1
Fagron	Clotrimazole	14C04-B31-299960	6
Caelo	Clotrimazole	14337812	6
Caelo	Clotrimazole	14337811	3
Caelo	Clotrimazole	14B05-B35	1
Noweda 07.07.2015	Clotrimazole	14144913	1
Fagron	Clotrimazole	14E26-B02	1
Fagron	Clotrimazole	14C04B31	1
Caelo	Clotrimazole	14B05-B36-291167	1
Caelo	Clotrimazole	143337811	1
Fagron	Clotrimazole	14B05B35294935	1
Noweda	Clotrimazole	1409027-02	1
Phoenix	Clotrimazole	14337812	1
Fagron	Clotrimazole	14C04-B32-291657	1
Noweda	Clotrimazole	14337801	1
Fagron	Clotrimazole	14B06-B06-299942	1
Fagron	Clotrimazole	14B05-B35-299941	2
Oberlinden Apotheke	Clotrimazole	201401300378	2
Caelo	Clotrimazole	14337809	13
Euro OTC	Clotrimazole	1409027-02Mg10g	1
Euro OTC	Clotrimazole	1409027-03	19
Fagron	Clotrimazole	1409027-02	1
Caelo	Clotrimazole	14337815	9
Caesar&Loretz GmbH/Anzag	Clotrimazole	14337807	1
Fagron	Clotrimazole	14B06-B06-299943	5
Caelo	Clotrimazole	14c04-b31-299954	2
Caelo	Clotrimazole	14C04B31-299954	1
Fagron	Clotrimazole	14b05-b35-299941	1
Caelo	Clotrimazole	1409027-03	3
Phönix Gotha	Clotrimazole	14337811	1
Caelo	Clotrimazole	14337813	6
Caello/Anzag	Clotrimazole	14337815	1
Caelo	Clotrimazole	14337816	14

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Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	14C04-B312-299959	1
Gehe	Clotrimazole	14337815	2
Caelo	Clotrimazole	14c04-B31	1
Euro OTC	Clotrimazole	1409027-04	26
AHD/Hedinger	Clotrimazole	14337807	1
Fagron	Clotrimazole	14C04-B31-299959	2
Bombastus	Clotrimazole	Validierungsmessung	1
Caelo	Clotrimazole	1437816	1
Fagron	Clotrimazole	14B06-B06	1
EuroTOC / Noweda	Clotrimazole	1409027-03	1
Fagron	Clotrimazole	15G14-B06-311055	1
Noweda	Clotrimazole	1409027	1
Fagron	Clotrimazole	14b05-b35-294935	1
Noweda	Clotrimazole	14337816	1
Caelo	Clotrimazole	14C04-B31-299955	1
Gehe	Clotrimazole	1409027-02	1
Caelo	Clotrimazole	14337814	8
Fagron	Clotrimazole	12E30-N02	1
Fagron	Clotrimazole	15G14-B06-311054	4
Caelo	Clotrimazole	14337817	12
Guangzhou Hanpu Pharmac...	Clotrimazole	1409027-03	1
Caelo	Clotrimazole	14337829	16
Sanacorp	Clotrimazole	14337817	1
Caelo	Clotrimazole	17011601	1
Caelo	Clotrimazole	14337824	3
Euro OTC	Clotrimazole	1510003-01	39
Anzag	Clotrimazole	15G14-B06	1
Caelo	Clotrimazole	15G14-B05-311101	1
Caelo	Clotrimazole	15G14-B06-311057	1
Caelo	Clotrimazole	1409027-04	1
Fagron	Clotrimazole	15G14B06311054	1
Caesar&Loretz GmbH	Clotrimazole	14337814	1
Fagron	Clotrimazole	15G14-B05-311101	1
Caelo	Clotrimazole	14337818	10
Euro OTC	Clotrimazole	15010003-01	1
Fagron	Clotrimazole	15G14-B06	1
Fagron	Clotrimazole	15G14-B05-311100	9
Euro OT/Gehe	Clotrimazole	1409027-03	2
Fagron	Clotrimazole	16B09-B06-311785	2
Noweda	Clotrimazole	1510003-01	2
Fagron	Clotrimazole	15G14-B05-311103	4
Fagron	Clotrimazole	16B09-B06-311507	4
Euro	Clotrimazole	1510003-01	2
Caelo	Clotrimazole	14337828	7
Euro OTC	Clotrimazole	140902703	1
Caelo	Clotrimazole	14337827	9
phönix	Clotrimazole	14337818	1
Fagron	Clotrimazole	15G14-Bo5-311101	1
Fagron	Clotrimazole	14337818	1
Caelo	Clotrimazole	14337832	1
Caelo	Clotrimazole	16B09-B06-311785	1
Caelo	Clotrimazole	15395602	13
apomix/Phönix	Clotrimazole	15G14-B05-311103	3
Caelo	Clotrimazole	14337819	6
Caelo	Clotrimazole	1510003-01	3
Caelo	Clotrimazole	14337830	2
Fagron	Clotrimazole	16B09-B06	1
Guangzhou Hanpu Pharmac...	Clotrimazole	1510003-01	1
Euro OTC	Clotrimazole	151000301	1
Euro OTC	Clotrimazole	140927-02	1

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Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	1510003-01	1
Caelo	Clotrimazole	15395604	10
wepa/Sanaco	Clotrimazole	14337819	1
Fagron	Clotrimazole	2616A-01276	1
Euro OTC	Clotrimazole	16B11-B04-320088	1
Fagron	Clotrimazole	15G14-B06-311056	1
Caelo	Clotrimazole	15395604	1
Euro OTC	Clotrimazole	1510003-02	14
Fagron	Clotrimazole	15G14-B05	4
Euro OTC	Clotrimazole	151003-01	1
Klenk	Clotrimazole	16B09-B06-311785	1
Caelo	Clotrimazole	15395603	9
Caelo	Clotrimazole	15395613	6
Fagron	Clotrimazole	16B09-B06-311506	2
Caelo	Clotrimazole	15G14-B05-316483	1
Caelo	Clotrimazole	15395605	11
Fagron	Clotrimazole	15G14-B06-31105	1
Euro OTC	Clotrimazole	151000	1
Euro OTC	Clotrimazole	1607046-01	44
Caelo	Clotrimazole	14B05-B36-291168	1
Caelo	Clotrimazole	141104C	1
Guangzhou Hanpu Pharmac...	Clotrimazole	1510003-02	1
Gehe	Clotrimazole	15G14-B05	1
Anzag	Clotrimazole	15395610	1
Caelo	Clotrimazole	15395611	8
Caelo	Clotrimazole	15395614	8
Euro OTC	Clotrimazole	160704601	4
Caesar u Loretz	Clotrimazole	15395613	1
Fagron	Clotrimazole	16E20-B10-321598	7
Caelo	Clotrimazole	15395615	3
Caelo	Clotrimazole	1607046-01	4
Hedinger/Alliance H.	Clotrimazole	15395617	1
Fagron	Clotrimazole	16B11-B04-320088	4
Fagron	Clotrimazole	15G14-B05-311102	3
Caelo	Clotrimazole	15295603	1
Caelo	Clotrimazole	15395617	8
Caelo	Clotrimazole	15395618	12
AHD 27.10 Ek.7,07	Clotrimazole	1607046	1
Caelo	Clotrimazole	16E20-B10	1
Bombastus	Clotrimazole	1607046-01	2
WE Phönix.01.12.2016 ...	Clotrimazole	15395618	1
Caelo	Clotrimazole	16234503	12
Fagron	Clotrimazole	16E20-B10-321597	2
Caelo	Clotrimazole	15395610	5
Fagron	Clotrimazole	16E20-B10-324555	1
Gehe	Clotrimazole	16E20-B10-321598	1
Alliance Healthcare	Clotrimazole	AP1510003-01C	1
caesar&loretz GmbH,Phön...	Clotrimazole	15395614	1
Euro OTC	Clotrimazole	1609046-01	1
Caelo	Clotrimazole	16234504	6
Caelo	Clotrimazole	AP1510003-01C	1
Fagron	Clotrimazole	16E20-B10-32197	1
Caesar & Loretz	Clotrimazole	16234504	1
Fagron	Clotrimazole	16E20-B10-326010	3
Euro OTC	Clotrimazole	H20160502	1
Fagron	Clotrimazole	CLT/1604/00227A	1
Euro OTC	Clotrimazole	1607046-0	1
Euro OTC	Clotrimazole	1607046-02	17
Caelo	Clotrimazole	16234505	12
Phönix	Clotrimazole	16234505	1

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Supplier	Substance	Batch	Spectra
Caesar u Loretz	Clotrimazole	16234501	1
Fagron	Clotrimazole	15G14-B05-316483	1
Klosterring	Clotrimazole	6234505	1
Noweda	Clotrimazole	15G14-B05-316483	2
Euro OTC	Clotrimazole	1607064-01	1
Caelo	Clotrimazole	16234501	5
Phönix	Clotrimazole	15395618	1
GEHE	Clotrimazole	1607046-02	1
Caelo	Clotrimazole	1623455	1
Fagron	Clotrimazole	CLT/1604/0027A	2
Caelo	Clotrimazole	160704601	1
Caelo	Clotrimazole	15395623	2
Caelo	Clotrimazole	16234511	12
Noweda/Apomix	Clotrimazole	15G14-B05-311100	1
apo ident	Clotrimazole	1607046-02	1
Euro	Clotrimazole	160704601	1
Caelo	Clotrimazole	16234513	12
Caelo	Clotrimazole	1607046-02	4
Euro/Noweda	Clotrimazole	1510003-02	1
Gehe	Clotrimazole	16234513	1
Fargon	Clotrimazole	16234511	1
Fagron	Clotrimazole	20170427Ma9	1
Caelo	Clotrimazole	16234509	6
Caelo	Clotrimazole	16234502	3
Euro OTC	Clotrimazole	1607046	1
Fagron	Clotrimazole	16B11-B04-327611	2
Euro OTC	Clotrimazole	160704602	1
Fagron	Clotrimazole	CLT/160/00058	1
Finteler Apotheke	Clotrimazole	16234501	1
Euro OTC	Clotrimazole	16234505	1
Euro OTC	Clotrimazole	1703028-01	44
Fargron / Noweda	Clotrimazole	16E20-B10-324555	1
Noweda	Clotrimazole	16234511	1
Caelo	Clotrimazole	16234506	1
Alliance/Euro	Clotrimazole	1703028-01	1
Fagron	Clotrimazole	16E20-B10-327349	5
Euro OTC	Clotrimazole	170615C/1703028-01	1
Euro OTC	Clotrimazole	170302801	3
Fagron	Clotrimazole	1703028-01	1
Fagron	Clotrimazole	17A19-B04332114	1
Caelo	Clotrimazole	16234512	9
Caelo	Clotrimazole	16234523	1
Audor Pharma	Clotrimazole	APCLT/1703/0016CC	2
Sanacorp	Clotrimazole	16E20-B10-327349	1
EuRho/ Phoenix	Clotrimazole	160704602	1
phoenix	Clotrimazole	16234512	1
Caelo	Clotrimazole	1170717	1
Euro OTC	Clotrimazole	20160801	3
Caelo	Clotrimazole	1703028-01	3
Sanacorp	Clotrimazole	15g14-b05-311100	1
Caelo	Clotrimazole	20160801	1
Caelo	Clotrimazole	162345135319	1
Fagron	Clotrimazole	16J07-B02-330216	2
Caelo	Clotrimazole	16234520	13
GEHE	Clotrimazole	16234513	1
EuRho / Phoenix	Clotrimazole	1703028-01	1
Fagron	Clotrimazole	16J07-B02-329385	1
Caelo	Clotrimazole	170302801	2
Fagron	Clotrimazole	3716Q-01276	1
Delta	Clotrimazole	1607046-01	1

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Supplier	Substance	Batch	Spectra
Caesar&Loretz GmbH,15.0...	Clotrimazole	16234509	1
Fagron	Clotrimazole	16J07-B02-329386	2
phönix	Clotrimazole	16234512	1
Noweda	Clotrimazole	16J07-B02-329386	1
Caelo	Clotrimazole	16234517	3
Finteler Apotheke	Clotrimazole	16234509	1
Caelo	Clotrimazole	16B11-B04-325221	1
Noweda	Clotrimazole	16234517	2
Anzag	Clotrimazole	1703028-01	1
Fagron	Clotrimazole	16234521	1
Caelo	Clotrimazole	16234521	4
Caelo	Clotrimazole	16J07-B02-329386	1
Caelo	Clotrimazole	16234522	6
Audor Pharma	Clotrimazole	APCLT/1703/0016C	1
Caelo	Clotrimazole	16234525	2
Klosterring	Clotrimazole	16234512	1
Caelo	Clotrimazole	2217Q-01276	1
Phönix WE:23.10.17 EK:...	Clotrimazole	16234521	1
Euro OTC	Clotrimazole	17A021	1
Caelo	Clotrimazole	17111604	3
Caelo	Clotrimazole	17111603	3
Sanacorp	Clotrimazole	16J07-B02-330216	1
Caelo	Clotrimazole	17111604	2
Caelo	Clotrimazole	17111605	8
Fagron	Clotrimazole	20171127Ma1	1
Caeolo/Gehe	Clotrimazole	16234521	1
Fagron	Clotrimazole	CLT/150570016b	1
Caelo	Clotrimazole	17111601	5
Fagron	Clotrimazole	16J07-B02-338283	2
Caelo	Clotrimazole	5117E-01276	1
Euro OTC	Clotrimazole	1703028-02	11
Fagron	Clotrimazole	17A19-SB04-332097	1
Caelo	Clotrimazole	17111606	7
Caelo	Clotrimazole	17111603	1
p&m cosmetics/gehe	Clotrimazole	16J07-B02-335773	2
Caelo	Clotrimazole	1711161	1
Cealo	Clotrimazole	17111612	1
Fagron	Clotrimazole	17A19-B04-334768	1
Caelo	Clotrimazole	17111616	7
Hedinger/Gehe	Clotrimazole	1703028-02	1
Euro OTC	Clotrimazole	150003-02	1
GEHE	Clotrimazole	177111613	1
Fagron	Clotrimazole	16J07-B02-340511	1
Sanacorp	Clotrimazole	16J07-B02-338283	1
Euro OTC	Clotrimazole	17111606	1
Caelo	Clotrimazole	1711816	1
Caelo	Clotrimazole	17111613	9
Caelo	Clotrimazole	1711613	1
Noweda	Clotrimazole	17111608	1
Gehe	Clotrimazole	1703028-02	1
Noweda/Fargon	Clotrimazole	17A19-B04-336568	1
Fagron	Clotrimazole	17A19-B04-340476	1
Caelo	Clotrimazole	17111615	6
Caelo	Clotrimazole	162345225555	1
Eurho	Clotrimazole	1703028-02	1
Fagron	Clotrimazole	16J07-B02-340513-201	1
Fagron	Clotrimazole	17J25-B06	1
Fagron	Clotrimazole	16J07-B02-335773	1
Fagron	Clotrimazole	14B05-B35-299944	1
Caelo	Clotrimazole	17111617	1

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Supplier	Substance	Batch	Spectra
Klosterring	Clotrimazole	17111615	2
Fagron	Clotrimazole	16J07-B02-340513	2
Fagron	Clotrimazole	17360201	1
Euro OTC	Clotrimazole	1703028-03	13
Caelo	Clotrimazole	17111608	7
AHD	Clotrimazole	1703028-03	1
Fagron	Clotrimazole	17J25-B06-345044	2
Fagron	Clotrimazole	16607-B02-333606	1
Caelo	Clotrimazole	17360201	14
Euro OTC	Clotrimazole	17360201	1
Sanacorp	Clotrimazole	17360203	1
Caelo	Clotrimazole	14337824NP	1
Caelo	Clotrimazole	17360202	8
Fagron	Clotrimazole	17A19-B04-338577	1
Caelo	Clotrimazole	171113608	1
Fagron	Clotrimazole	17J25-B06-345407	1
Fagron	Clotrimazole	17A19-B04-336568	1
Sanacorp	Clotrimazole	17360201	1
Fagron	Clotrimazole	18A18-B05-344819	1
Caelo	Clotrimazole	17360204	3
Fagron	Clotrimazole	18A18-B05-347865	2
Fagron	Clotrimazole	17J25-B06-347476	2
Caelo	Clotrimazole	170302803	1
Caelo	Clotrimazole	17360203	3
Caelo	Clotrimazole	17A19-B04-340476	1
Fagron	Clotrimazole	18A18-B05-348429	1
Bombastus	Clotrimazole	17360203	1
Fagron	Clotrimazole	CLT/1711/0077A	1
Fagron	Clotrimazole	17J25-B06-349161	2
Caelo	Clotrimazole	18147206	1
Caelo	Clotrimazole	18147103	6
Caelo	Clotrimazole	18147101	8
Caelo/GEHE	Clotrimazole	18147101	2
Fagron	Clotrimazole	1A1-B05-34765	1
Caelo	Clotrimazole	18147203	5
Caelo	Clotrimazole	181471035763	1
Euro OTC	Clotrimazole	170302802	1
Euro OTC	Clotrimazole	1808028-01	9
euro//Noweda	Clotrimazole	1808028-01	1
Kehr	Clotrimazole	1808028-01	1
Fagron	Clotrimazole	16J07-B02-344818	1
Caelo	Clotrimazole	18147208	1
Sanacorp	Clotrimazole	18147102	1
Fagron	Clotrimazole	18G10-B06-353348	1
Fagron	Clotrimazole	700135-0003	1
Euro OTC	Clotrimazole	1808028	1
Caelo	Clotrimazole	18147102	3
Sanacorp	Clotrimazole	18147212	1
Euro OTC	Clotrimazole	1808028-02	1
Fagron	Clotrimazole	18A18-B05-352115	1
Caelo	Clotrimazole	18081408	1
Fagron	Clotrimazole	18G10-B06-352708	1

- 77 093 spectra from 565 *Apo-Ident* customers from a total of 25 751 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#),

the samples are listed in the *Type C* section of each substance page. If the substance 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* can clearly be 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* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	74 136
Type B	0	290	0	126 602
Type C	0	1805	31	77 093

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.9310 %)
Type C	100.0000 % (> 99.8817 %)	98.3115 % (> 98.1481 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20794	23791	3.42	45.81
21087	23791	3.43	43.53
21114	23791	3.05	42.39
21207	23791	7.48	39.89
21259	23791	7.00	43.11
21264	22229	5.99	41.55
21352	23791	3.59	42.66
22229	22229	0.00	43.85
23791	23791	0.00	43.21

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Colistin sulfate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20318-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Colistin sulfate; Colistin sulphate; Colistini sulfas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Colistin sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Colistin sulfate	13G05-N01	20915	40	20130719
Fagron	Colistin sulfate	14E02-B03	21346	40	1501654
Euro OTC	Colistin sulfate	1406001-01	21619	40	1508600
Euro OTC	Colistin sulfate	1507044	21852	40	20150817*
Euro OTC	Colistin sulfate	1602021	22371	40	20160307*
Euro OTC	Colistin sulfate	1606008	22695	40	20160704*
Fagron	Colistin sulfate	16F03-B01-324216	22973	40	20160706

Validation samples

A total of 280317 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 *Colistin sulfate*. These samples are listed above in the [calibration samples](#) section.
- 74216 spectra from a total of 1616 batches from further 372 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 [†].

- 345 spectra of 10 reference samples from the substance/substance group *Colistin sulfate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Colistin sulfate	13G05-N01	21209	40
Euro OTC	Colistin sulfate	1406001-01	21619 [†]	20
Euro OTC	Colistin sulfate	1406002-01	21700	45
Euro OTC	Colistin sulfate	1507044	21852 [†]	20
Euro OTC	Colistin sulfate	1602021	22371 [†]	20
Audor Pharma	Colistin sulfate	APKB-CS-1602026C	22974	40
Audor Pharma	Colistin sulfate	APKB-CS-1603034C	23026	40
Audor Pharma	Colistin sulfate	APKB-CS-1602026C	23027	40
Euro OTC	Colistin sulfate	1709009	23616	40
Euro OTC	Colistin sulfate	1710041	23866	40

- 126547 spectra from a total of 2780 batches from further 781 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.

- 8 spectra from 4 *Apo-Ident* customers from 7 batches from the substance/substance group *Colistin sulfate*.

Supplier	Substance	Batch	Spectra
Euro OTC	Colistin sulfate	1507044-01	1
Fagron	Colistin sulfate	15E15-B01-315340	1
Audor Pharma	Colistin sulfate	APKB-CS-1601026C	1
Caelo	Colistin sulfate	1602021-01	1
Audor Pharma	Colistin sulfate	APKB-CS-1603034C	2
Audor Pharma	Colistin sulfate	APKB-CS-1610012C	1
Fagron	Colistin sulfate	16F03-B01	1

- 78 921 spectra from 565 *Apo-Ident* customers from a total of 26 130 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Colistin sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Colistin sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 216
Type B	0	294	51	126 547
Type C	0	7	1	78 921

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	85.2174 % (> 84.3478 %)
Type C	100.0000 % (> 99.8818 %)	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
21346	21346	0.00	20.36
22695	22695	0.00	25.45
20915	22371	3.89	23.18
22371	22371	0.00	22.91
21619	21619	0.00	25.71
21852	21852	0.00	23.27
22973	21852	1.02	23.20

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Colophony
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20627-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Colophony; Colophonium

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Colophony*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Colophony	12301410	21782	40	AR-15-FG-016314-01
Caelo	Colophony	15186804	21971	40	AR-16-FG-005931-01
Caelo	Colophony	161332	22588	40	20160510*

Validation samples

A total of 280 317 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 *Colophony*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Colophony*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Colophony	12301410	21782 [†]	20
Caelo	Colophony	15186804	21971 [†]	20
Caelo	Colophony	173014	23794	40
Caelo	Colophony	173014	24052	40

- 126 772 spectra from a total of 2786 batches from further 781 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 4 *Apo-Ident* customers from 1 batches from the substance/substance group *Colophony*.

*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	Colophony	15186807	8

- 78 921 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Colophony* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Colophony* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	40	80	126 772
Type C	0	2	6	78 921

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	33.3333 % (> 30.8333 %)
Type C	100.0000 % (> 99.8818 %)	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
21971	21971	0.00	39.60
21782	21782	0.00	110.11
22588	22588	0.00	71.08

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Cyanocobalamin / Ethinylestradiol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20950-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Cyanocobalamin / Ethinylestradiol; Cyanocobalamin; Cyanocobalaminum; Ethinylestradiol; Ethinylestradiolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Cyanocobalamin / Ethinylestradiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ethinylestradiol	13I09-N04	20950	40	1402058
Caelo	Cyanocobalamin	13342803	21299	40	AR-15-FG-005429-01
Caelo	Cyanocobalamin	13342807	21479	40	AR-15-FG-014917-01
Euro OTC	Cyanocobalamin	1305040-01	21635	40	AR-15-FG-005214-01

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ethinylestradiol	14E15-B03-296049	21705	40	1507109
Euro OTC	Cyanocobalamin	1506035	21867	40	20150708*
Euro OTC	Cyanocobalamin	1506035	21872	40	0000010479
Fagron	Ethinylestradiol	14E15-B03-310270	21916	40	20140708
Caelo	Cyanocobalamin	160154	22441	40	20160309*
Euro OTC	Cyanocobalamin	1604017	22536	30	20160509*
Caelo	Cyanocobalamin	13342807	21479SI	20	AR-15-FG-014917-01
Fagron	Ethinylestradiol	14E15-B03-296049	21705SI	36	1507109
Euro OTC	Cyanocobalamin	1506035	21867SI	40	20150708*
Euro OTC	Cyanocobalamin	1506035	21872SI	30	0000010479
Fagron	Ethinylestradiol	14E15-B03-310270	21916SI	40	20140708
Caelo	Cyanocobalamin	160154	22441SI	40	20160309*
Euro OTC	Cyanocobalamin	1604017	22536SI	30	20160509*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 626 spectra of 17 reference samples from the substance/substance group *Cyanocobalamin* / *Ethinylestradiol*. These samples are listed above in the [calibration samples](#) section.
- 73 870 spectra from a total of 1614 batches from further 371 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 [†].

- 573 spectra of 21 reference samples from the substance/substance group *Cyanocobalamin* / *Ethinylestradiol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cyanocobalamin	09351704	20858	40
Caelo	Cyanocobalamin	13342807	21479 [†]	20
Euro OTC	Cyanocobalamin	1305040-01	21635 [†]	20
Fagron	Ethinylestradiol	14E15-B03-296049	21705 [†]	15
Euro OTC	Cyanocobalamin	1506035	21867 [†]	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	Cyanocobalamin	1506035	21872 [†]	20
Fagron	Ethinylestradiol	14E15-B03-310270	21916 [†]	20
Fagron	Ethinylestradiol	14E15-B03-310270	21958	60
Caelo	Cyanocobalamin	160154	22441 [†]	20
Fagron	Ethinylestradiol	16B17-B01-329904	23075	40
Caelo	Cyanocobalamin	16015411	23761	40
Caelo	Cyanocobalamin	162215	23790	40
Caelo	Cyanocobalamin	13342807	21479SI [†]	40
Fagron	Ethinylestradiol	14E15-B03-296049	21705SI [†]	20
Euro OTC	Cyanocobalamin	1506035	21867SI [†]	20
Euro OTC	Cyanocobalamin	1506035	21872SI [†]	15
Fagron	Ethinylestradiol	14E15-B03-310270	21916SI [†]	20
Fagron	Ethinylestradiol	14E15-B03-310270	21958SI	43
Caelo	Cyanocobalamin	160154	22441SI [†]	20
Euro OTC	Cyanocobalamin	1604017	22536SI [†]	10
Fagron	Ethinylestradiol	16B17-B01-329904	23075SI	30

- 126 319 spectra from a total of 2778 batches from further 780 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.

- 21 spectra from 18 *Apo-Ident* customers from 18 batches from the substance/substance group *Cyanocobalamin* / *Ethinylestradiol*.

Supplier	Substance	Batch	Spectra
Fagron	Ethinylestradiol	13I09-N04	1
Fagron	Ethinylestradiol	13G03-N04	1
Fagron	Ethinylestradiol	12D19-N04	1
Fagron	Ethinylestradiol	14e15b03296049	1
Fagron	Ethinylestradiol	84100720	1
Fagron	Ethinylestradiol	16B17-B01	1
Fagron	Ethinylestradiol	16B17-B01-320666	1
Euro OTC	Cyanocobalamin	5061204	1
Caesar & Loretz GmbH, 4...	Cyanocobalamin	9324102	1
Caelo	Cyanocobalamin	9373503	2
Fagron	Cyanocobalamin	10K02-N05	1
Caelo	Cyanocobalamin	9324113	1
Fagron	Cyanocobalamin	10K02-N05	2
Caelo	Cyanocobalamin	9351704	1
Caelo	Cyanocobalamin	9324102	1
Fagron	Cyanocobalamin	13124-B01-292062	1
Fagron	Cyanocobalamin	15H31-B02-315113	1
Caelo	Cyanocobalamin	1604017-01	1
Fagron	Cyanocobalamin	17A27-B04	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*.

- 78 908 spectra from 565 *Apo-Ident* customers from a total of 26 119 batches from a further 692 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	626	0	73 870
Type B	0	528	45	126 319
Type C	0	15	6	78 908

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 99.0415 %)
Type B	100.0000 % (> 99.9901 %)	92.1466 % (> 91.6230 %)
Type C	100.0000 % (> 99.8817 %)	71.4286 % (> 57.1429 %)

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
20950	20950	0.00	21.33
21635	21635	0.00	16.61
21867	21867	0.00	13.53
21916	21705	7.64	21.40
21872	21872	0.00	22.20
21479	21479	0.00	16.76

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21299	21299	0.00	14.98
21705	21705	0.00	23.93
22441	22441	0.00	27.34
22536	22536	0.00	29.06

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Cyproterone acetate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20593-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Cyproterone acetate; Cyproteroni acetat

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Cyproterone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cyproterone acet...	13C11-N02	21262	40	1501534
Fagron	Cyproterone acet...	13J16-No4	21985	55	1602654
Fagron	Cyproterone acet...	15I11-B01-322117	22665	40	20150921
Euro OTC	Cyproterone acet...	1611003	22875	40	20161201*
Fagron	Cyproterone acet...	17D11-B07-333693	23238	40	20170501
Fagron	Cyproterone acet...	17D11-B07-333693	23238SI	20	20170501

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 235 spectra of 6 reference samples from the substance/substance group *Cyproterone acetate*. These samples are listed above in the [calibration samples](#) section.
- 74261 spectra from a total of 1618 batches from further 372 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 [†].

- 286 spectra of 10 reference samples from the substance/substance group *Cyproterone acetate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cyproterone acetate	13J16-No4	21985 [†]	20
Audor Pharma	Cyproterone acetate	APCPA140201CP	23988	40
Fagron	Cyproterone acetate	18G25-B02-352728	24289	40
Euro OTC	Cyproterone acetate	1810017	24317	40
Fagron	Cyproterone acetate	13J16-No4	21985SI	23
Fagron	Cyproterone acetate	15I11-B01-322117	22665SI	33
Euro OTC	Cyproterone acetate	1611003	22875SI	30
Audor Pharma	Cyproterone acetate	APCPA140201CP	23988SI	20
Fagron	Cyproterone acetate	18G25-B02-352728	24289SI	20
Euro OTC	Cyproterone acetate	1810017	24317SI	20

- 126606 spectra from a total of 2783 batches from further 781 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.

- 31 spectra from 22 *Apo-Ident* customers from 23 batches from the substance/substance group *Cyproterone acetate*.

Supplier	Substance	Batch	Spectra
Fagron	Cyproterone acetate	11L22-N02	1
Fagron	Cyproterone acetate	12L19-N05	2
Fagron	Cyproterone acetate	B0392/110020	3
Fagron	Cyproterone acetate	12F25-N09	2
Fagron	Cyproterone acetate	12D02-N13	1
Fagron	Cyproterone acetate	12J24-N02	1
Fagron	Cyproterone acetate	13/16-N04	2
Fagron	Cyproterone acetate	13/09-N03	1
Fagron	Cyproterone acetate	8B11-N06	1
Fagron	Cyproterone acetate	13J16-N04	2
Fagron	Cyproterone acetate	13j16n04	1
Fagron	Cyproterone acetate	13j16-no4	1
Caelo	Cyproterone acetate	13j16-n04	1
Audor Pharma	Cyproterone acetate	APCPA140201CP	1
Fagron	Cyproterone acetate	15I11-B01-315381	2
Fagron	Cyproterone acetate	16K09-B04-329037	1
Fagron	Cyproterone acetate	EU-CPA-170301	1
Ebert-Jacobi	Cyproterone acetate	16K09-B04-329036	1
Caelo	Cyproterone acetate	17D11-B07-334581	2
Audor Pharma	Cyproterone acetate	cpa140201cp	1
Fagron	Cyproterone acetate	17D11-B07-338440	1
Fagron	Cyproterone acetate	17D11-B07	1
Sanacorp	Cyproterone acetate	18B05-B05-346307	1

- 78 898 spectra from 565 *Apo-Ident* customers from a total of 26 114 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Cyproterone 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 *Cyproterone 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	235	0	74 261
Type B	0	274	12	126 606
Type C	0	19	12	78 898

The substance/substance group *Cyproterone 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 % (> 99.9887 %)	100.0000 % (> 97.4468 %)
Type B	100.0000 % (> 99.9901 %)	95.8042 % (> 94.7552 %)
Type C	100.0000 % (> 99.8817 %)	61.2903 % (> 51.6129 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21985	21985	0.00	57.50
22665	21985	2.07	56.95
21262	21262	0.00	57.44
22875	22875	0.00	56.53
23238	21985	1.67	56.39

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Cystine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20515-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Cystine; Cystinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Cystine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cystine	1307052-01	21328	40	20130918
Euro OTC	Cystine	1408016-01	21715	40	20140911
Euro OTC	Cystine	1603010	22523	40	20160406*
Euro OTC	Cystine	1610013	22863	40	20161110*
Euro OTC	Cystine	1801016	23879	40	20180126*

Validation samples

A total of 280317 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 *Cystine*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 *Cystine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cystine	1408016-01	21715 [†]	20
Fagron	Cystine	15F08-B05-310685	23767	40
Euro OTC	Cystine	1811005	24332	40

- 126792 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 12 spectra from 5 *Apo-Ident* customers from 9 batches from the substance/substance group *Cystine*.

*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	Cystine	1207013-01	2
Euro OTC	Cystine	2081301	1
Euro OTC	Cystine	1204090	1
Fagron	Cystine	12D26-B04-285823	2
Euro OTC	Cystine	26081408	1
Euro OTC	Cystine	3021502	1
Euro OTC	Cystine	30041809	1
Euro OTC	Cystine	1801016-01	2
Fagron	Cystine	15F08-B05-310685	1

- 78 917 spectra from 565 *Apo-Ident* customers from a total of 26 128 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Cystine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cystine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	100	0	126 792
Type C	0	12	0	78 917

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8818 %)	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
21328	22523	3.30	42.80
21715	22523	4.23	43.01
22523	22523	0.00	43.07
22863	22863	0.00	43.45
23879	23879	0.00	42.87

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Dapsone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22489-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dapsone; Dapsonum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Dapsone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dapsone	160735	22489	40	20160405*
Caelo	Dapsone	170311	23301	39	20170221*

Validation samples

A total of 280 317 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 *Dapsone*. These samples are listed above in the [calibration samples](#) section.
- 74 417 spectra from a total of 1621 batches from further 372 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 *Dapsone*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dapsone	160735	22489 [†]	20
Caelo	Dapsone	16073502	22577	40
Caelo	Dapsone	16073502	22736	40
Caelo	Dapsone	182792	24400	40

- 126 752 spectra from a total of 2786 batches from further 781 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 *Dapsone*.

*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*.

- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Dapsone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dapsone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 417
Type B	0	140	0	126 752
Type C	0	0	0	78 929

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.4051 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.8817 %)	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
22489	22489	0.00	94.38
23301	23301	0.00	93.93

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Dequalinium chloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20350-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dequalinium chloride; Dequalinii chloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Dequalinium chloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Dequalinium chlo...	13I26-N10	21269	40	20130121
Caelo	Dequalinium chlo...	12361908	21296	40	1412076
Caelo	Dequalinium chlo...	12361906	21387	40	20121228
Euro OTC	Dequalinium chlo...	1405012-01	21617	40	20140623
Euro OTC	Dequalinium chlo...	1512032	22295	40	20160121*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dequalinium chlo...	15218406	22953	40	20150622
Caelo	Dequalinium chlo...	15402803	23121	40	1707614
Fagron	Dequalinium chlo...	15B16-B04-332113	23266	40	20150226
Caelo	Dequalinium chlo...	154028	23362	40	20160219*
Euro OTC	Dequalinium chlo...	1512032-02	24142	40	1809202

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Dequalinium chloride*. These samples are listed above in the [calibration samples](#) section.
- 74 096 spectra from a total of 1613 batches from further 372 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 †.

- 780 spectra of 16 reference samples from the substance/substance group *Dequalinium chloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Dequalinium chloride	11D29-N11	20660	80
Caelo	Dequalinium chloride	12077503	20716	40
Caelo	Dequalinium chloride	12361906	21386	60
Caelo	Dequalinium chloride	12361906	21387†	80
Euro OTC	Dequalinium chloride	1405012-01	21617†	20
Euro OTC	Dequalinium chloride	1512032	22295†	20
Caelo	Dequalinium chloride	180794	24011	40
Euro OTC	Dequalinium chloride	1804009	24082	40
Caelo	Dequalinium chloride	154028	24403	40
Caelo	Dequalinium chloride	12361906	21386SI	60
Caelo	Dequalinium chloride	12361906	21387SI	60
Euro OTC	Dequalinium chloride	1405012-01	21617SI	60
Euro OTC	Dequalinium chloride	1512032	22295SI	60
Caelo	Dequalinium chloride	15218406	22953SI	40
Fagron	Dequalinium chloride	15B16-B04-332113	23266SI	40
Caelo	Dequalinium chloride	154028	23362SI	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.

- 126 112 spectra from a total of 2779 batches from further 781 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.

- 147 spectra from 105 *Apo-Ident* customers from 66 batches from the substance/substance group *Dequalinium chloride*.

Supplier	Substance	Batch	Spectra
Euro OTC	Dequalinium chloride	1103045-01	1
Euro OTC	Dequalinium chloride	15061204	1
Anzag ek:7.89EUR	Dequalinium chloride	11166204	1
Euro OTC	Dequalinium chloride	1110002-01	2
Fagron	Dequalinium chloride	12G05-N07	2
Caelo	Dequalinium chloride		1
Noweda	Dequalinium chloride	12b14-n05	1
EuRho	Dequalinium chloride	1110002-01	1
Caelo	Dequalinium chloride	11166209	1
Caelo	Dequalinium chloride	11166203	1
Fagron	Dequalinium chloride	12D05-N09	1
Caelo	Dequalinium chloride	12G05-N07	1
Euro OTC	Dequalinium chloride	1210008-01	1
Caelo	Dequalinium chloride	12077508	2
Caelo	Dequalinium chloride	11166204	2
Alliance Health	Dequalinium chloride	12077508	1
Fagron	Dequalinium chloride	13A23-N02	3
Euro OTC	Dequalinium chloride	1010022-01	2
Euro OTC	Dequalinium chloride	1210008-02	2
Caelo	Dequalinium chloride	12077510	7
Fagron	Dequalinium chloride	13D26-N06	3
Phönix	Dequalinium chloride	10127-N02Retest	1
Euro OTC	Dequalinium chloride	1210008-03	2
Caelo	Dequalinium chloride	220812K2	1
S.Binder	Dequalinium chloride	1210008-04	1
Caelo	Dequalinium chloride	12361906	3
LEBSA/Phoenix	Dequalinium chloride	1210008-03	1
Caelo	Dequalinium chloride	1210008-03	1
Fagron	Dequalinium chloride	10H05-N07	1
Caelo	Dequalinium chloride	12361908	2
Raben-Apotheke Mildenau	Dequalinium chloride	1405012-01	1
Caelo	Dequalinium chloride	12361911	3
Euro OTC	Dequalinium chloride	1405012-01	5
Lebsa/AHD	Dequalinium chloride	1405012-01	1
Fagron	Dequalinium chloride	14C10-B03	1
Caelo	Dequalinium chloride	3613A-01325	1
Caelo	Dequalinium chloride	1405012-02	1
Fagron	Dequalinium chloride	13I26-N10	1
Fagron	Dequalinium chloride	14C10-B03-292286	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
Euro OTC	Dequalinium chloride	1405012-02	3
Caelo	Dequalinium chloride	13A23-N02	1
Caelo	Dequalinium chloride	13348805	2
Caelo	Dequalinium chloride	15218401	6
Caelo	Dequalinium chloride	14072901	1
Caelo	Dequalinium chloride	14C10-B03	1
Euro OTC	Dequalinium chloride	1407029-01	7
Fagron	Dequalinium chloride	15B16-B04-304432	1
Fagron	Dequalinium chloride	1407029-01	2
Caelo	Dequalinium chloride	15218402	1
Caelo	Dequalinium chloride	215I-01325	1
Caelo	Dequalinium chloride	15218404	2
Lamotte/Spangroh	Dequalinium chloride	15218404	1
Caelo	Dequalinium chloride	13/26-N10	1
Fagron	Dequalinium chloride	12B14-N01	1
Fagron	Dequalinium chloride	15B16B04304432	1
Euro OTC	Dequalinium chloride	1407029-02	4
Caelo	Dequalinium chloride	15218407	1
Caelo	Dequalinium chloride	15218406	2
Euro OTC	Dequalinium chloride	151203201	1
Caelo	Dequalinium chloride	15218410	1
Euro OTC	Dequalinium chloride	1512032-01	12
Caelo	Dequalinium chloride	5315I-01325	1
Fag / Noweda	Dequalinium chloride	15B16-B04-321326	1
Klosterring	Dequalinium chloride	15B16-B04-321326	1
Phönix	Dequalinium chloride	151203201	1
Allianz Healthcare	Dequalinium chloride	1512032-01	1
Fagron	Dequalinium chloride	15B16-B04-316267	2
Fagron	Dequalinium chloride	15B16-B04	1
Gehe	Dequalinium chloride	1512032-01	1
Fagron	Dequalinium chloride		1
Euro OTC	Dequalinium chloride	11091701	1
Caelo	Dequalinium chloride	15402803	1
Fagron	Dequalinium chloride	15B16-B04-326872	1
Caelo	Dequalinium chloride	15402801	1
Fagron	Dequalinium chloride	15B16-B04-340177	1
Caelo	Dequalinium chloride	15402805	1
Caelo	Dequalinium chloride	15B16-B04-342302	1
Anzag	Dequalinium chloride	15B16-B04-340177	1
Euro OTC	Dequalinium chloride	1512032-02	2
Caelo	Dequalinium chloride	18015802	1
Fagron	Dequalinium chloride	15B16-B04-342302	1
Caelo	Dequalinium chloride	18015801	1
Euro/Sanacorp	Dequalinium chloride	1512032-02	1
Fagron	Dequalinium chloride	15B16-B04-346969	2
Caelo	Dequalinium chloride	18079402	1
Caelo	Dequalinium chloride	18079403	1

- 78 782 spectra from 565 *Apo-Ident* customers from a total of 26 071 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	400	0	74 096
Type B	0	673	107	126 112
Type C	0	111	36	78 782

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9901 %)	86.2821 % (> 85.8974 %)
Type C	100.0000 % (> 99.8817 %)	75.5102 % (> 73.4694 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22295	22295	0.00	41.61
23121	23121	0.00	54.21
23266	23362	12.59	46.28
23362	23362	0.00	43.54
21269	21296	23.59	43.57
21387	21296	9.38	41.56
22953	21296	20.13	42.14
24142	24142	0.00	67.12
21296	21296	0.00	32.56
21617	21296	9.90	42.15

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Dexamethasone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20009-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dexamethasone; Dexamethasonum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Dexamethasone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Dexamethasone	1303007-01	21289	40	1407432
Caelo	Dexamethasone	13084315	21403	40	AR-15-FG-006810-01
Euro OTC	Dexamethasone	1601052	22364	30	20160225*
Euro OTC	Dexamethasone	1611001	22914	40	20161212*
Fagron	Dexamethasone	16F02-B05-324844	23168	40	20160711
Euro OTC	Dexamethasone	1601052	22364SI	30	20160225*
Euro OTC	Dexamethasone	1611001	22914SI	37	20161212*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 257 spectra of 7 reference samples from the substance/substance group *Dexamethasone*. These samples are listed above in the [calibration samples](#) section.
- 74 239 spectra from a total of 1618 batches from further 372 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 [†].

- 648 spectra of 18 reference samples from the substance/substance group *Dexamethasone*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dexamethasone	13084306	21062	60
Euro OTC	Dexamethasone	1209008-02	21078	60
Caelo	Dexamethasone	13084315	21403 [†]	20
Euro OTC	Dexamethasone	1303007-01	21850	60
Euro OTC	Dexamethasone	1601052	22364 [†]	15
Caelo	Dexamethasone	15054627	23169	40
Caelo	Dexamethasone	171042	23331	40
Euro OTC	Dexamethasone	1708004	23692	40
Caelo	Dexamethasone	172856	23841	40
Euro OTC	Dexamethasone	1806023	24136	40
Euro OTC	Dexamethasone	1303007-01	21850SI	45
Euro OTC	Dexamethasone	1601052	22364SI [†]	15
Fagron	Dexamethasone	16F02-B05-324844	23168SI	30
Caelo	Dexamethasone	15054627	23169SI	20
Caelo	Dexamethasone	171042	23331SI	24
Euro OTC	Dexamethasone	1708004	23692SI	26
Caelo	Dexamethasone	172856	23841SI	40
Euro OTC	Dexamethasone	1806023	24136SI	33

*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*.

- 126 244 spectra from a total of 2778 batches from further 781 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.

- 684 spectra from 278 *Apo-Ident* customers from 177 batches from the substance/substance group *Dexamethasone*.

Supplier	Substance	Batch	Spectra
Euro OTC	Dexamethasone	1107006-01	1
Caesar & Loretz GmbH, 4. . .	Dexamethasone	10369922	1
Fagron	Dexamethasone	11F30-N02	1
Euro OTC	Dexamethasone	1111055-01	5
Phoenix	Dexamethasone	10369928	1
Caelo	Dexamethasone	10369921	2
Euro OTC	Dexamethasone	111105501	1
Fagron	Dexamethasone	12D26-N09	2
Euro OTC	Dexamethasone		1
Caelo	Dexamethasone	10369920	8
Caelo	Dexamethasone	12033301	3
Euro OTC	Dexamethasone	1111055-02	2
Fagron	Dexamethasone	11L08-N01	4
Euro OTC	Dexamethasone	1512211327	1
Caelo	Dexamethasone	12033305	4
Euro OTC	Dexamethasone	DZ11005K	1
Caelo	Dexamethasone	9383631	1
Gehe	Dexamethasone	1203032-02	1
Anzag	Dexamethasone	1233305	1
Fagron	Dexamethasone	12H21-N11	2
Euro OTC	Dexamethasone	1203032-01	4
Caelo	Dexamethasone	12033308	2
Fagron	Dexamethasone	12B06-N12	2
Caelo	Dexamethasone	12165803	1
Noweda	Dexamethasone	12033307	2
Caelo	Dexamethasone	12033307	4
Caelo	Dexamethasone	12033304	1
Sanofi-Chimie, FR/ Noweda	Dexamethasone	12033308	1
Euro OTC	Dexamethasone	1203032-02	3
Fagron	Dexamethasone	1209008-01	1
Caelo	Dexamethasone	12033314	7
Caelo	Dexamethasone	12033318	4
Caelo	Dexamethasone	12033312	2
Caelo	Dexamethasone	12033315	4
Caelo	Dexamethasone	12033317	5
Euro OTC	Dexamethasone	1209008-01	10
Caelo	Dexamethasone	13084305	4
Euro OTC	Dexamethasone	1209008-02	25
Caelo	Dexamethasone	12091306	1
Pharmacia&Upjohn Comp	Dexamethasone	1209008-02	1
Caelo	Dexamethasone	13084304	1
Euro OTC	Dexamethasone	120900802	2
Caelo	Dexamethasone	13084310	8
Fagron	Dexamethasone	13D12-N09	3

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Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone	3084310	1
Euro OTC	Dexamethasone	5213A1327	1
Phönix	Dexamethasone	12033314	1
Caelo	Dexamethasone	13084308	2
Euro OTC	Dexamethasone	130300701	4
Fagron	Dexamethasone	DZ11005K12B06-N12	1
Caelo	Dexamethasone	13084307	2
Caelo	Dexamethasone	13084306	3
Fagron	Dexamethasone	13G08-N13	3
Phönix Gotha	Dexamethasone	12033315	1
Caelo	Dexamethasone	130854306	1
Caelo	Dexamethasone	13D12-N09	1
Caelo	Dexamethasone	13G08-N13	2
Caelo	Dexamethasone	13084309	1
GEHE 12.03.2014	Dexamethasone	13084306	1
Caelo	Dexamethasone	13084313	2
Phoenix	Dexamethasone	13084313	2
Gehe 8.04.2014	Dexamethasone	13084310	2
Caelo	Dexamethasone	13084316	3
Caelo	Dexamethasone	13084317	5
Gehe	Dexamethasone	13084317	1
Sanacorp	Dexamethasone	13084308	1
Caelo	Dexamethasone	13084320	2
Caelo	Dexamethasone	13352302	8
Euro OTC	Dexamethasone	1303007-01	29
Henry Lamotte Oils GmbH	Dexamethasone	13084304	1
Caelo	Dexamethasone	13084319	4
Fagron	Dexamethasone	11D26-N10	3
Raben-Apotheke Mildenau	Dexamethasone	1303007-01	2
Fagron	Dexamethasone	2314A-01327	1
Phoenix	Dexamethasone	13g08n13	1
Fagron	Dexamethasone	13D12-N19	1
Euro OTC	Dexamethasone	13030007-01	1
Fagron	Dexamethasone	14A22-B03	2
Euro OTC	Dexamethasone	14D11-B01-294031	1
Euro OTC	Dexamethasone	13030007	1
Caelo	Dexamethasone	13352310	12
Phoenix Goettin	Dexamethasone	117113352302	1
Euro OTC	Dexamethasone	DB003/0213	3
Caelo	Dexamethasone	13352309	1
Caesar & Loretz/Noweda	Dexamethasone	13084319	1
Symbiotica	Dexamethasone	1303007-01	1
Fagron	Dexamethasone	14A22-B03-294030	1
Fagron	Dexamethasone	14A22-B03-290701	1
Euro OTC	Dexamethasone	130300702	2
Sanacorp	Dexamethasone	13352309	1
Phönix Gotha	Dexamethasone	13352311	1
Euro OTC	Dexamethasone	1303007-02	9
Caelo	Dexamethasone	13352308	4
Caelo	Dexamethasone	13352311	1
Caelo	Dexamethasone	13352312	11
Caelo	Dexamethasone	13352304	1
Caelo	Dexamethasone	13352315	2
Caelo	Dexamethasone		3
Euro OTC	Dexamethasone	1303007-03	26
Fagron	Dexamethasone	15A05-B01-034636	1
Caleo	Dexamethasone	15054602	2
Euro OTC	Dexamethasone	1303007	1
Caelo	Dexamethasone	13342310	1
Euro OTC	Dexamethasone	13352309	1

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Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone	14196402	3
Fagron	Dexamethasone	15A05-B01-304636	3
Gehe	Dexamethasone	15054602	2
Caelo	Dexamethasone	1335213	1
Fagron	Dexamethasone	13L30-B34-289691	1
Caelo	Dexamethasone	15054602	4
Caelo	Dexamethasone	15054606	10
Caelo	Dexamethasone	1303007-03	1
Noweda	Dexamethasone	1303007-03	1
Caelo	Dexamethasone	15054605	5
Fagron	Dexamethasone	1303007-03	1
Sanofi-Chimie FR/Noweda	Dexamethasone	15054606	2
Fagron	Dexamethasone	15A05-B01	1
Caelo	Dexamethasone	15054611	4
Caelo	Dexamethasone	15054603	1
Fagron	Dexamethasone	15C16-B07-308252	1
Symbiotica	Dexamethasone	1303007-03	2
Caelo	Dexamethasone	15054609	3
Caesar&Loretz GmbH,Phön...	Dexamethasone	15054606	2
Fagron	Dexamethasone	15054603	1
Caelo	Dexamethasone	15A05-B01-304637	1
Euro OTC	Dexamethasone	130300703	1
Fagron	Dexamethasone	14D11-B01-294032	1
Caelo	Dexamethasone	1504610	1
Fagron	Dexamethasone	15I04-B04-315528	1
Euro OTC	Dexamethasone	1601052-01	19
Caelo	Dexamethasone	15054617	8
Phoenix	Dexamethasone	15I04-B04	1
Caelo	Dexamethasone	15054618	2
Fagron	Dexamethasone	15/04-B04-315528	1
unbekannt	Dexamethasone	12D26-N09	1
Caelo	Dexamethasone	15215601	1
Caelo	Dexamethasone	15054610	1
Caelo	Dexamethasone	160821D	1
Fagron	Dexamethasone	15C16-B07	1
Fagron	Dexamethasone	15K17-B07-321457	1
Euro OTC	Dexamethasone	160105201	2
Fagron	Dexamethasone	15054614	1
Euro OTC	Dexamethasone	1601052-02	25
Euro OTC	Dexamethasone	700107	1
Caesar & Loretz GmbH	Dexamethasone	15054622	1
Euro/ Sanacorp	Dexamethasone	1601052-01	2
Caelo	Dexamethasone	15054622	17
EuRho / Phoenix	Dexamethasone	1303007-03	1
Caelo	Dexamethasone	15054623	5
Fagron	Dexamethasone	15A05-B01-304637	1
Fagron	Dexamethasone	16I06-B03-327323	1
ALH	Dexamethasone	15054617	2
Fagron	Dexamethasone	14D11-B01-294031	1
Pharmacia&Upjohn Compan...	Dexamethasone	1601052-02	1
PHÖNIX	Dexamethasone	15K17-B07	1
Symbiotica/Noweda	Dexamethasone	1601052-02	1
EuRho Anzag	Dexamethasone	1601052-02	1
Caelo	Dexamethasone	15054621	6
caesar&loretz GmbH,Phön...	Dexamethasone	15054622	3
Caelo	Dexamethasone	15054616	2
Caelo	Dexamethasone	1601052-02	1
Fagron	Dexamethasone	16/06-B03-327323	1
caesar	Dexamethasone	15054617	1
Euro OTC	Dexamethasone	15054621	1

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Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone	15054620/170314D	1
Euro OTC	Dexamethasone	1611001-01	28
Caelo	Dexamethasone	15054628	8
Fagron	Dexamethasone	700107-0002	1
Gehe	Dexamethasone	15054621	1
Noweda/Apomix	Dexamethasone	1611001-01	1
Fagron	Dexamethasone	16I06-B03-327488	3
Euro OTC	Dexamethasone	161100101	2
Gehe	Dexamethasone	15054629	1
Euro OTC	Dexamethasone	L53613	1
Ebert-Jacobi	Dexamethasone	1611001-01	1
Sanacorp	Dexamethasone	1601052-01	1
Caelo	Dexamethasone	15054627	2
Fagron	Dexamethasone	16K24B05330281	1
Fagron	Dexamethasone	17C13-B07-332461	1
Caelo	Dexamethasone	15054631	2
Caelo	Dexamethasone	17104204	2
PH Euro 8,0	Dexamethasone	15054610	1
Caelo	Dexamethasone	1504631	1
Caelo	Dexamethasone	15054629	5
Caelo	Dexamethasone	16012207	1
Noweda	Dexamethasone	17104204	1
Euro OTC	Dexamethasone	17104204	1
Fagron	Dexamethasone	17104203	1
Euro OTC	Dexamethasone	1611001	1
EuRho / Phoenix	Dexamethasone	15054631	1
Bombastus	Dexamethasone	150546629	1
Caelo	Dexamethasone	1704203	1
Caelo	Dexamethasone	17104205	2
Caelo	Dexamethasone	1611001-01	2
Caelo	Dexamethasone	1704204	1
Fagron	Dexamethasone	17E31-B01-338016	1
Caelo	Dexamethasone	17081716	1
Caelo	Dexamethasone	17104203	3
Caelo	Dexamethasone	17104211	8
Caelo	Dexamethasone	17104210	6
Caelo	Dexamethasone	1714203	1
Euro OTC	Dexamethasone	1708004-01	24
Euro/Gehe	Dexamethasone	1611001-01	1
Euro OTC	Dexamethasone	180208D/1611001-01	1
Fagron	Dexamethasone	17E31-B01-331860	1
Caelo	Dexamethasone	171042165511	1
Caelo	Dexamethasone	17104216	2
Kehr	Dexamethasone	17104205	1
Kehr	Dexamethasone	17104210	1
Caelo	Dexamethasone	17104212	1
Euro OTC	Dexamethasone	1702004-01	1
Euro OTC	Dexamethasone	1303007-04	1
Caelo	Dexamethasone	17332403	6
Caelo	Dexamethasone	171042165585	1
Anzag	Dexamethasone	17332404	1
Euro OTC	Dexamethasone	T45290	1
Fagron	Dexamethasone	17L19-B03-344100	2
Fagron	Dexamethasone	NUD160702	1
AHD	Dexamethasone	17L19-B03-344099	1
Sanacorp	Dexamethasone	17332402	1
Caelo	Dexamethasone	17332402	3
Caelo	Dexamethasone	17332404	7
calo	Dexamethasone	17332403	1
Caelo	Dexamethasone	16K24-B05-330281	1

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Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone	17332406	3
Fagron	Dexamethasone	17L19-B03-344396	1
Krieger	Dexamethasone	17332406	1
Caelo	Dexamethasone	17332412	4
Caelo	Dexamethasone	17332404	1
Caelo	Dexamethasone	17332414	4
Caelo	Dexamethasone	17332413	2
Caelo	Dexamethasone	1708004-01	1
Caelo	Dexamethasone	17332408	2
Euro OTC	Dexamethasone	1806023-01	2
Caelo	Dexamethasone	17332415	1
Caelo	Dexamethasone	17332411	1
Caelo	Dexamethasone	17332415-D20180115Ma	1
Caelo	Dexamethasone	17332419	4
Caelo	Dexamethasone	17332407	1

- 78 245 spectra from 565 *Apo-Ident* customers from a total of 25 964 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	257	0	74 239
Type B	0	624	24	126 244
Type C	0	652	32	78 245

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.6654 %)
Type B	100.0000 % (> 99.9901 %)	96.2963 % (> 95.8333 %)
Type C	100.0000 % (> 99.8817 %)	95.3216 % (> 94.8830 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22914	22914	0.00	12.85
23168	21289	5.48	59.84
21403	21403	0.00	10.73
22364	22364	0.00	12.71
21289	21289	0.00	56.47

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Dexamethasone acetate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20313-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dexamethasone acetate; Dexamethasoni acetat

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Dexamethasone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dexamethasone ac...	13260703	21301	40	1412430
Caelo	Dexamethasone ac...	13260706	21593	40	1502537
Euro OTC	Dexamethasone ac...	1405024-01	21614	40	20140620
Caelo	Dexamethasone ac...	14200207	21815	40	20140807
Euro OTC	Dexamethasone ac...	1405024-01	21614SI	30	20140620
Caelo	Dexamethasone ac...	14200207	21815SI	30	20140807

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 6 reference samples from the substance/substance group *Dexamethasone acetate*. These samples are listed above in the [calibration samples](#) section.
- 74276 spectra from a total of 1619 batches from further 372 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 [†].

- 316 spectra of 11 reference samples from the substance/substance group *Dexamethasone acetate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dexamethasone acetate	13260706	21593 [†]	20
Euro OTC	Dexamethasone acetate	1405024-01	21614 [†]	20
Caelo	Dexamethasone acetate	14200207	21815 [†]	20
Caelo	Dexamethasone acetate	161066	22437	60
Euro OTC	Dexamethasone acetate	1708011	23693	40
Caelo	Dexamethasone acetate	181730	24253	40
Euro OTC	Dexamethasone acetate	1405024-01	21614SI [†]	15
Caelo	Dexamethasone acetate	14200207	21815SI [†]	15
Caelo	Dexamethasone acetate	161066	22437SI	42
Euro OTC	Dexamethasone acetate	1708011	23693SI	24
Caelo	Dexamethasone acetate	181730	24253SI	20

- 126576 spectra from a total of 2783 batches from further 781 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](#).

[†]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.

- 138 spectra from 67 *Apo-Ident* customers from 63 batches from the substance/substance group *Dexamethasone acetate*.

Supplier	Substance	Batch	Spectra
Euro OTC	Dexamethasone acetate	1110007-01	2
Caelo	Dexamethasone acetate	11093211	1
Caelo	Dexamethasone acetate	12021803	3
Caelo	Dexamethasone acetate	11093210	1
Caelo	Dexamethasone acetate	11093215	1
EuRho	Dexamethasone acetate	1110007-01	1
Caelo	Dexamethasone acetate	12021811	1
Caelo	Dexamethasone acetate	12021814	2
Caelo	Dexamethasone acetate	12021801	2
Caelo	Dexamethasone acetate	5/AD1	1
Euro OTC	Dexamethasone acetate	1110007-02	5
Caelo	Dexamethasone acetate	13100403	5
Caelo	Dexamethasone acetate	3913Q-01326	1
Caelo	Dexamethasone acetate	4113I-01326	1
Caelo	Dexamethasone acetate	13100401	1
Caelo	Dexamethasone acetate	13100404	2
Caelo	Dexamethasone acetate	13100407	4
Caelo	Dexamethasone acetate	13100406	1
Caelo	Dexamethasone acetate	22/AKD2	1
europharma	Dexamethasone acetate	1110007-01	1
Caelo	Dexamethasone acetate	13100408	2
Noweda	Dexamethasone acetate	13100406	1
Caelo	Dexamethasone acetate	13260703	3
Fagron	Dexamethasone acetate	1110007	1
Caelo	Dexamethasone acetate	13260705	1
Euro OTC	Dexamethasone acetate	1110007-03	1
Caelo	Dexamethasone acetate	13260701	3
Noweda	Dexamethasone acetate	1110007-02	1
Caelo	Dexamethasone acetate	14200201	2
Caelo	Dexamethasone acetate	1405024-01	1
Caelo	Dexamethasone acetate	14200205	2
Euro OTC	Dexamethasone acetate	1405024-02	6
Caelo	Dexamethasone acetate	13260702	1
Caelo	Dexamethasone acetate	14200207	1
Caelo	Dexamethasone acetate	14200208	1
Euro OTC	Dexamethasone acetate	140502402	1
Euro OTC	Dexamethasone acetate	1405024-03	12
Caelo	Dexamethasone acetate	15243202	3
Caelo	Dexamethasone acetate	140502403	1
Caelo	Dexamethasone acetate	14379602	1
Caelo	Dexamethasone acetate	14379609	3
Caelo	Dexamethasone acetate	14379611	1
Euro OTC	Dexamethasone acetate	1405024-04	1
Apomix/AHD	Dexamethasone acetate	1405024-03	1
Caelo	Dexamethasone acetate	14379607	1
Euro OTC	Dexamethasone acetate	1405024-01	1
Caelo	Dexamethasone acetate	14379616	4
Caelo	Dexamethasone acetate	15243201	1
Caelo	Dexamethasone acetate	14379601	1
Caelo	Dexamethasone acetate	16106602	1
Caelo	Dexamethasone acetate	14379615	4
Caelo	Dexamethasone acetate	16106604	1

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Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone acetate	14379608	1
Caelo	Dexamethasone acetate	16106608	3
Caelo	Dexamethasone acetate	16106607	3
Caelo	Dexamethasone acetate	16106603	3
Caelo	Dexamethasone acetate	16106603/171025DM	1
Caelo	Dexamethasone acetate	16106613	4
Caelo	Dexamethasone acetate	16106610	1
Phönix	Dexamethasone acetate	16106603	1
Caelo	Dexamethasone acetate	16106611	1
Caelo	Dexamethasone acetate	16106616	5
Caelo	Dexamethasone acetate	16106612	1
Euro OTC	Dexamethasone acetate	1708011-01	4
Sanacorp	Dexamethasone acetate	16106613	1
Caelo	Dexamethasone acetate	16106619	1
Caelo	Dexamethasone acetate	161066165624	1
Caelo	Dexamethasone acetate	16106623	1
Caelo	Dexamethasone acetate	18173002	1
Sanofi Chimie/ Gehe	Dexamethasone acetate	18173004	1
Caelo	Dexamethasone acetate	16106615	1
Caelo	Dexamethasone acetate	18173004	1

- 78 791 spectra from 565 *Apo-Ident* customers from a total of 26 074 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Dexamethasone 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 *Dexamethasone 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	220	0	74 276
Type B	0	309	7	126 576
Type C	0	119	19	78 791

The substance/substance group *Dexamethasone 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 % (> 99.9887 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9901 %)	97.7848 % (> 96.8354 %)
Type C	100.0000 % (> 99.8817 %)	86.2319 % (> 84.0580 %)

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

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

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21593	21593	0.00	28.51
21301	21301	0.00	22.16
21614	21301	1.03	21.37
21815	21593	8.79	24.25

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Dextromethorphan hydrobromide monohydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	22318-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dextromethorphan hydrobromide monohydrate; Dextromethorphan hydrobromidum

Special notes

When selecting the *Dextromethorphan hydrobromide monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Dextromethorphan hydrobromide monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Dextromethorphan...	15D23-B07-308849	22318	40	AR-16-FG-008487-02
Fagron	Dextromethorphan...	16A22-B03-321371	23103	40	20160205
Fagron	Dextromethorphan...	17B28-B01-341594	23780	40	20170612

Validation samples

A total of 280 317 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 *Dextromethorphan hydrobromide monohydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Dextromethorphan hydrobromide monohydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Dextromethorphan hydrobromid...	15D23-B07-308849	22318 [†]	20
Fagron	Dextromethorphan hydrobromid...	15D23-B07-308849	22326	60
Fagron	Dextromethorphan hydrobromid...	16E23-B02-329706	23593	40
Fagron	Dextromethorphan hydrobromid...	18B09-B02-350261	24288	40

- 126 732 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 13 spectra from 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Dextromethorphan hydrobromide monohydrate*.

[†]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
Fagron	Dextromethorphan hydrobromid. ...	14H27-B04-299502	7
Fagron	Dextromethorphan hydrobromid. ...	16A22-B03-321371	5
Fagron	Dextromethorphan hydrobromid. ...	16A22-B03-319331	1

- 78 916 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Dextromethorphan hydrobromide monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dextromethorphan hydrobromide monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	0	126 732
Type C	0	13	0	78 916

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8818 %)	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
22318	22318	0.00	45.50
23103	22318	3.16	44.93
23780	22318	6.57	44.72

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **D-galactose**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20326-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

D-galactose; D-Galactopyranose

Special notes

When selecting the *D-galactose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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-galactose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Falcento	D-galactose	007223PF3	20894	40	20130128
Fagron	D-galactose	13I13-B40-287993	21762	40	AR-15-FG-008936-01
Fagron	D-galactose	14H05-B09-310972	22259	40	20140818

Validation samples

A total of 280 317 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 *D-galactose*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *D-galactose*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	D-galactose	11F30-N08	20839	40
Fagron	D-galactose	13I13-B40-287993	21762 [†]	20
Fagron	D-galactose	14H05-B09-310972	22259 [†]	20
Fagron	D-galactose	15G13-B04-320810	23106	40
Fagron	D-galactose	15G13-B04-320810	23595	40

- 126 732 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 31 spectra from 3 *Apo-Ident* customers from 24 batches from the substance/substance group *D-galactose*.

[†]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
Falcento	D-galactose	10440003	1
Phönix	D-galactose	39223PF3	1
Falcento	D-galactose	2014	1
Phönix 04.03.2014	D-galactose		1
Falcento	D-galactose	122PF4	1
Falcento	D-galactose	1223PF4	3
Falcento	D-galactose	2223PF4	3
Falcento	D-galactose	222PF4	1
Falcento	D-galactose	5223PF4	3
Falcento	D-galactose	12223PF4	2
Falcento	D-galactose	13223PF4	1
inalco	D-galactose	212619PF5	1
falcento	D-galactose	322619PF5	1
Unisan	D-galactose	432619PF5	1
Unisan	D-galactose	382619PF5	1
Unisan	D-galactose	442619PF5	1
Falcento	D-galactose	233619PF5	1
Falcento	D-galactose	92619PF64744/16	1
Falcento	D-galactose	82619PF64743/16	1
Fagron	D-galactose	16G22-B01-329906	1
Falcento	D-galactose	82619PF7	1
Falcento	D-galactose	72619PF7	1
inalco	D-galactose	32619PF8	1
inalco	D-galactose	42619PF4	1

- 78 898 spectra from 565 *Apo-Ident* customers from a total of 26 113 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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-galactose* can clearly be 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-galactose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	0	126 732
Type C	0	30	1	78 898

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	96.7742 % (> 87.0968 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21762	21762	0.00	43.87
22259	21762	5.00	44.51
20894	21762	10.34	44.52

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Diclofenac sodium**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20022-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Diclofenac sodium; Diclofenacum natricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Diclofenac sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Diclofenac sodium	12214219	20883	20	20120815
Fagron	Diclofenac sodium	13E03-N02	20886	40	20130515
Fagron	Diclofenac sodium	12L28-B05	21261	40	20130123
Caelo	Diclofenac sodium	13214311	21467	40	20130826
Caelo	Diclofenac sodium	13214311	21470	40	20130826
Euro OTC	Diclofenac sodium	1607016	22694	40	20160808*
Caelo	Diclofenac sodium	163492	23037	40	20170112*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 7 reference samples from the substance/substance group *Diclofenac sodium*. These samples are listed above in the [calibration samples](#) section.
- 74 236 spectra from a total of 1617 batches from further 372 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 *Diclofenac sodium*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Diclofenac sodium	1403013-01	21330	40
Caelo	Diclofenac sodium	13214311	21467 [†]	20
Caelo	Diclofenac sodium	13214311	21470 [†]	20
Fagron	Diclofenac sodium	15D14-B04-307452	21979	60
Euro OTC	Diclofenac sodium	1711026	23872	40

- 126 712 spectra from a total of 2785 batches from further 781 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*.

- 209 spectra from 97 *Apo-Ident* customers from 78 batches from the substance/substance group
Diclofenac sodium.

Supplier	Substance	Batch	Spectra
Noweda	Diclofenac sodium	11G12-N06	1
Caelo	Diclofenac sodium	11091201	1
Euro OTC	Diclofenac sodium	13111203	1
Euro OTC	Diclofenac sodium	1111040-01	2
Europharm/Otto	Diclofenac sodium	135796	1
Caelo	Diclofenac sodium	12214205	1
Euro OTC	Diclofenac sodium	1206026-01	6
Caelo	Diclofenac sodium	12214206	1
Sanacorp	Diclofenac sodium	1206026-01	1
Euro OTC	Diclofenac sodium	1206026-02	3
Caelo	Diclofenac sodium	12214219	1
Euro OTC	Diclofenac sodium	1206026	1
Fagron	Diclofenac sodium	13E03-N02	1
Fagron	Diclofenac sodium	14031411	1
Caelo	Diclofenac sodium	13214304	1
Fagron	Diclofenac sodium	5041401	1
Caelo	Diclofenac sodium	12214202	1
Caelo	Diclofenac sodium	13214303	1
Caelo	Diclofenac sodium	13214309	3
Caelo	Diclofenac sodium	13214308	2
Euro OTC	Diclofenac sodium	1403013-01	4
Euro OTC	Diclofenac sodium	140301301	1
Euro OTC	Diclofenac sodium	12214220	1
Caelo	Diclofenac sodium	13214311	8
Euro OTC	Diclofenac sodium	1403013-02	6
Fagron	Diclofenac sodium	12L28-B05-289773	2
Fagron	Diclofenac sodium	RDS/1405/0159A	1
Caelo	Diclofenac sodium	140301301	1
Fargron	Diclofenac sodium	14G17-B08-297032	1
Fagron	Diclofenac sodium	14G17-B08-297032	6
Caelo	Diclofenac sodium	13214312	2
EurRho/ Anzag	Diclofenac sodium	1403013-03	1
Fischar/Phönix	Diclofenac sodium	13214311	1
Caelo	Diclofenac sodium	13214317	5
Caelo	Diclofenac sodium	12L28-B05	1
Euro OTC	Diclofenac sodium	1403013-03	3
Fagron	Diclofenac sodium	14G17B08297032	1
Caelo	Diclofenac sodium	13214316	1
Caelo	Diclofenac sodium	13214318	3
Noweda	Diclofenac sodium	1403013-01	1
Phönix	Diclofenac sodium	1403013-03	1
Fagron	Diclofenac sodium	15D14-B04	1
Euro OTC	Diclofenac sodium	1503014-01	10
Caelo	Diclofenac sodium	1503014-01	1
Euro OTC	Diclofenac sodium	12060250	1
Caelo	Diclofenac sodium	15169604	6
Euro OTC	Diclofenac sodium	1503014-02	4
Fagron	Diclofenac sodium	15D14-B04-314450	3
Fagron	Diclofenac sodium	15D14-B04-315835	1
AHD	Diclofenac sodium	15D14B04314450	1
Fagron	Diclofenac sodium	15K23-B03-318519	2
Fagron	Diclofenac sodium	15K23-B03	1
Fagron	Diclofenac sodium	15K23-B03-321673	2
Fagron	Diclofenac sodium		1
Sanacorp	Diclofenac sodium	3616Q-02994	1
Caelo	Diclofenac sodium	15K23-B03-318519	2
Fagron	Diclofenac sodium	15K23-B03-324025	3

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Supplier	Substance	Batch	Spectra
Caelo	Diclofenac sodium	15169675	1
Caelo	Diclofenac sodium	15169615	1
Euro OTC	Diclofenac sodium	1607016-01	17
Caelo	Diclofenac sodium	15169609	1
Fagron	Diclofenac sodium	15K23-B03-325753	3
Phoenix	Diclofenac sodium	15K23-B03	1
Fargon GmbH & Co.KG	Diclofenac sodium	15K23-B03-325753	1
Fagron	Diclofenac sodium	15K23-B03-327802	4
siehe Protokoll	Diclofenac sodium	15169617	1
Caelo	Diclofenac sodium	15K23-B03-325753	1
Gehe	Diclofenac sodium	15278502	1
Euro OTC	Diclofenac sodium	1607016-02	6
Caelo	Diclofenac sodium	15169613	1
Caelo	Diclofenac sodium	15278505	2
Caelo	Diclofenac sodium	15278502	2
Fagron	Diclofenac sodium	16I29-B04-332372	2
Caelo	Diclofenac sodium	15278506	2
Hedinger/Phoenix	Diclofenac sodium	15278506	3
Euro OTC	Diclofenac sodium	15169606	1
Euro OTC	Diclofenac sodium	1607016-03	14
Noweda	Diclofenac sodium	15278504	1
Fagron	Diclofenac sodium	17F02-B05	1
Caelo	Diclofenac sodium	15278507	1
Fagron	Diclofenac sodium	16129	1
Fagron	Diclofenac sodium	17F02	1
Fagron	Diclofenac sodium	17F02-B05-338797	4
Euro OTC	Diclofenac sodium	1711026-01	3
Bombastus	Diclofenac sodium	1711026-01	1
Noweda	Diclofenac sodium	18039202	1
Fagron	Diclofenac sodium	17j19-B01-342310	1
Caelo	Diclofenac sodium	16349207	1
Caelo	Diclofenac sodium	18039202	1
Caelo	Diclofenac sodium	18039203	1
Euro OTC	Diclofenac sodium	1711026-1	1
EuRho/Spangro	Diclofenac sodium	1711026-02	2
Kehr	Diclofenac sodium	1711026-03	1

- 78 720 spectra from 565 *Apo-Ident* customers from a total of 26 059 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Diclofenac sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diclofenac sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 236
Type B	0	180	0	126 712
Type C	0	206	3	78 720

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	98.5646 % (> 97.1292 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20883	23037	6.16	60.32
20886	23037	13.72	60.85
21261	23037	11.00	60.60
21467	23037	6.04	58.48
21470	23037	5.38	61.52
22694	22694	0.00	68.23
23037	23037	0.00	59.67

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Diltiazem hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20043-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Diltiazem hydrochloride; Diltiazemi hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Diltiazem hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Diltiazem hydroc...	14C12-B04	21270	40	20140417
Caelo	Diltiazem hydroc...	13346914	21300	40	20131028
Caelo	Diltiazem hydroc...	161908	22631	40	20160715*
Fagron	Diltiazem hydroc...	16G20-B03-328133	23016	40	20160829

Validation samples

A total of 280 317 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 *Diltiazem hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 [†].

- 280 spectra of 6 reference samples from the substance/substance group *Diltiazem hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Diltiazem hydrochloride	13346914	21406	60
Caelo	Diltiazem hydrochloride	13346914	21407	60
Fagron	Diltiazem hydrochloride	16G20-B03-328133	23015	40
Caelo	Diltiazem hydrochloride	170432	23325	40
Caelo	Diltiazem hydrochloride	173370	23826	40
Caelo	Diltiazem hydrochloride	183011	24389	40

- 126 612 spectra from a total of 2784 batches from further 781 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.

- 1127 spectra from 363 *Apo-Ident* customers from 284 batches from the substance/substance group *Diltiazem hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	11E18-N04	3
Caelo	Diltiazem hydrochloride	11134117	4
Fiebig ek:12.27 01.08.12	Diltiazem hydrochloride	11/01-N08	1
Sanacorp	Diltiazem hydrochloride	11134121	2
Fagron	Diltiazem hydrochloride	12D05-N070	1
Fagron	Diltiazem hydrochloride	12d05-n07	1
Caelo	Diltiazem hydrochloride	12133006	1
Caelo	Diltiazem hydrochloride	12177101	13
Caelo	Diltiazem hydrochloride	11L20-N06	1
Fagron	Diltiazem hydrochloride	12D05-N07	13
Caelo	Diltiazem hydrochloride	12176801	1
Fagron	Diltiazem hydrochloride	10D28-N23	1
Caelo	Diltiazem hydrochloride	2310213562	1
Noweda	Diltiazem hydrochloride	12176801	1
Sanacorp	Diltiazem hydrochloride	11134115	4
Fagron	Diltiazem hydrochloride	612213562	1
Fagron	Diltiazem hydrochloride	11-01-N08	1
Gehe	Diltiazem hydrochloride	12133009	1
Caelo	Diltiazem hydrochloride	DIL/M-04511	1
Caelo	Diltiazem hydrochloride	12133009	7
Fagron	Diltiazem hydrochloride	12F19-N10	3
Fagron	Diltiazem hydrochloride	12I12-N02	2
Fagron	Diltiazem hydrochloride	12/12-N02	4
Caelo	Diltiazem hydrochloride	10212413	1
Fagron	Diltiazem hydrochloride	11I01-N08	1
Caelo	Diltiazem hydrochloride	12176804	1
Noweda	Diltiazem hydrochloride	12133010	1
Caelo	Diltiazem hydrochloride	12133011	3
Caelo	Diltiazem hydrochloride	12133010	11
Caelo	Diltiazem hydrochloride	12/12-N02	1
Sanacorp	Diltiazem hydrochloride	11J28-04511	1
Caelo	Diltiazem hydrochloride	6031302	1
Fagron	Diltiazem hydrochloride	12/12-N02	1
Caelo	Diltiazem hydrochloride	12133008	2
Caesar & Loretz GmbH	Diltiazem hydrochloride	12133010	1
phoenix	Diltiazem hydrochloride	11/01-N08	1
Sanacorp	Diltiazem hydrochloride	12I12-N02	1
Alliance	Diltiazem hydrochloride	12133009	1
Caelo	Diltiazem hydrochloride	12133014	2
Sanacorp	Diltiazem hydrochloride	12133010	1
Alliance Healthcare	Diltiazem hydrochloride	12I12-N02	1
Caelo	Diltiazem hydrochloride	12133022	10
Fagron	Diltiazem hydrochloride	12K07-N02	2
Caelo	Diltiazem hydrochloride	10069509	1
Fagron	Diltiazem hydrochloride	13A02-N05	7
Caelo	Diltiazem hydrochloride	12133028	4
Noweda	Diltiazem hydrochloride	12133022	1
Caelo	Diltiazem hydrochloride	12133029	3
Piramal Healthcare Ltd...	Diltiazem hydrochloride	12/12-N02	1
Piramal Healthcare LTD.	Diltiazem hydrochloride	12F19-N10	1
Sanacorp	Diltiazem hydrochloride	12/12-N02	2
Caelo	Diltiazem hydrochloride	12133023	1
Alliance Health	Diltiazem hydrochloride	13A02-N05	1
Fagron	Diltiazem hydrochloride	10808-N01	1
Gehe	Diltiazem hydrochloride	12133022	1
Fagron	Diltiazem hydrochloride	13F13-N05	9
Caelo	Diltiazem hydrochloride	10212404	1

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Supplier	Substance	Batch	Spectra
Alliance	Diltiazem hydrochloride	12133008	1
Noweda	Diltiazem hydrochloride	12133029	1
Caelo	Diltiazem hydrochloride	3313U-03562	1
Phönix	Diltiazem hydrochloride	13F13-N05	1
Caelo	Diltiazem hydrochloride	DIL/M-19911	1
Fagron	Diltiazem hydrochloride	12F19-N100102/574	1
Fagron	Diltiazem hydrochloride	13a02-n05	1
Fagron	Diltiazem hydrochloride	13A02N05	3
Caelo	Diltiazem hydrochloride	1319604	1
Caelo	Diltiazem hydrochloride	13196104	7
Caelo	Diltiazem hydrochloride	11091301	1
Caelo	Diltiazem hydrochloride	13196107	3
Fagron	Diltiazem hydrochloride	3713M-03562	1
Caelo	Diltiazem hydrochloride	13196105	16
Caelo	Diltiazem hydrochloride	1396103	1
Fagron	Diltiazem hydrochloride	13G16-N05	22
Caelo	Diltiazem hydrochloride	13196103	2
Caelo	Diltiazem hydrochloride	11134113	1
Caelo	Diltiazem hydrochloride	13G16-No5	1
Caelo	Diltiazem hydrochloride	13346901	8
Caelo	Diltiazem hydrochloride	1334609	1
Caelo	Diltiazem hydrochloride	13346904	5
Caelo	Diltiazem hydrochloride	13A02-N05	1
Caelo	Diltiazem hydrochloride	13j24-b04-286571	1
Caelo	Diltiazem hydrochloride	13346905	9
Fagron	Diltiazem hydrochloride	12112-N02	1
Fagron	Diltiazem hydrochloride	13J24B04286569	3
Caelo	Diltiazem hydrochloride	13346902	4
Caelo	Diltiazem hydrochloride		1
Fagron	Diltiazem hydrochloride	13346902	1
Fagron	Diltiazem hydrochloride	13J24-B04-286569	11
Fagron	Diltiazem hydrochloride	9J14-N17	1
Fagron	Diltiazem hydrochloride	13J24-B04-286571	2
Fagron	Diltiazem hydrochloride	11J28-N05	1
Caelo	Diltiazem hydrochloride	13346903	9
Sanacorp	Diltiazem hydrochloride	13j24-b04-286569	1
Noweda	Diltiazem hydrochloride	13346901	1
Fagron	Diltiazem hydrochloride	13J24-B04	3
Phönix	Diltiazem hydrochloride	13196106	1
Fagron	Diltiazem hydrochloride	13j24-b04-286569	1
Caelo	Diltiazem hydrochloride	13J24-B04-286569	1
Phoenix	Diltiazem hydrochloride	13346902	1
Caelo	Diltiazem hydrochloride	25041401	1
Caelo	Diltiazem hydrochloride	13G16-N05	1
Fagron	Diltiazem hydrochloride	13J24-B04-286570	1
Caelo	Diltiazem hydrochloride	13346908	1
Phoenix	Diltiazem hydrochloride	13346914	1
Fagron	Diltiazem hydrochloride	14C12-B04-292757	22
Caelo	Diltiazem hydrochloride	13346914	5
Caelo	Diltiazem hydrochloride	13J24-B04-289432	3
Fagron	Diltiazem hydrochloride	14C12-B04	7
Caelo	Diltiazem hydrochloride	14059502	1
Caelo	Diltiazem hydrochloride	13346915	8
Fagron	Diltiazem hydrochloride	13346915	1
AHD	Diltiazem hydrochloride	14C12-B04-292757	1
Fagron	Diltiazem hydrochloride	14C12-B04-292759	4
Caelo	Diltiazem hydrochloride	14059504	3
11.08.14 Phoenix	Diltiazem hydrochloride	13346901	1
Fagron	Diltiazem hydrochloride	22082014A	1
Anzag	Diltiazem hydrochloride	13346915	1

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Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	DIL/M-0314	1
Caelo	Diltiazem hydrochloride	1405904	1
Caelo	Diltiazem hydrochloride	14059514	15
Kuerzel	Diltiazem hydrochloride	13G16-N05	1
Caelo	Diltiazem hydrochloride	14059521	2
Fagron	Diltiazem hydrochloride	14C12B04	1
Gehe	Diltiazem hydrochloride	14C12-B04-292757	1
Caelo	Diltiazem hydrochloride	14059513	17
Fagron	Diltiazem hydrochloride	14c12-b04-292759	1
Caelo	Diltiazem hydrochloride	14059503	3
Apomix/Noweda	Diltiazem hydrochloride	14C12-B04-292759	1
Caelo	Diltiazem hydrochloride	23121402	1
Fagron	Diltiazem hydrochloride	DIL/M-01314	1
Fagron	Diltiazem hydrochloride	14C12B04-294133	1
Fagron	Diltiazem hydrochloride	14C12-B04-294133	4
Caelo	Diltiazem hydrochloride	14059515	2
Fagron	Diltiazem hydrochloride	14c12-b04-294134	1
Fagron	Diltiazem hydrochloride	14C12-B04-294134	1
Caelo	Diltiazem hydrochloride	14C12-B04-294133	1
phönix	Diltiazem hydrochloride	14059514	1
Caelo	Diltiazem hydrochloride	14318403	4
Caelo	Diltiazem hydrochloride	14318402	4
Fagron	Diltiazem hydrochloride	135968-0009	2
Caelo	Diltiazem hydrochloride	13031501	1
Caelo	Diltiazem hydrochloride	14318409	13
Caelo	Diltiazem hydrochloride	140595143	1
Caelo	Diltiazem hydrochloride	14C12-B04-294135	1
Sanacorp	Diltiazem hydrochloride	14c12-b04-292757	1
VDL;18.02.15;15,95EUR	Diltiazem hydrochloride	14059514	1
Fagron	Diltiazem hydrochloride	14C12B04292757	1
Caelo	Diltiazem hydrochloride	14059133	1
Fagron	Diltiazem hydrochloride	14G22-B08-299781	11
Caelo	Diltiazem hydrochloride	14318410	3
Fagron	Diltiazem hydrochloride	14G22-B08-299782	6
Caelo	Diltiazem hydrochloride	14318412	17
Sanacop	Diltiazem hydrochloride	14059523	1
Cealo/Sanacorp	Diltiazem hydrochloride	14059514	1
Fagron	Diltiazem hydrochloride	14G22-B08299781	2
Fagron	Diltiazem hydrochloride	14G22-B08	3
Fagron	Diltiazem hydrochloride	14G22-B08-299783	1
Gehe	Diltiazem hydrochloride	14G22-B08-299781	1
phoenix	Diltiazem hydrochloride	14318412	1
Caesar&Loretz GmbH/Anzag	Diltiazem hydrochloride	14318412	1
Caelo	Diltiazem hydrochloride	14G22-B08-299781	1
Caelo	Diltiazem hydrochloride	18061511	1
Caelo	Diltiazem hydrochloride	14318413	3
Fagron	Diltiazem hydrochloride	15B12-B01-305399	21
Fagron	Diltiazem hydrochloride	15b12-b01-305399	2
Caelo	Diltiazem hydrochloride	14318416	2
sittig	Diltiazem hydrochloride	14G22-B08-299781	1
Noweda	Diltiazem hydrochloride	14318409	1
Caelo	Diltiazem hydrochloride	14g22b08299781	1
Caelo	Diltiazem hydrochloride	15/246/DI	1
Caelo	Diltiazem hydrochloride	15212801	7
Caelo	Diltiazem hydrochloride	15212802	7
Fagron	Diltiazem hydrochloride	15B12-B01305399	1
Fagron	Diltiazem hydrochloride	15B12-B01	5
Caelo	Diltiazem hydrochloride	1091503	1
Fagron	Diltiazem hydrochloride	15B12B01305399	2
Fagron	Diltiazem hydrochloride	14G22B08	1

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Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	DIL/M-13114	1
Caelo	Diltiazem hydrochloride	14318414	2
Fagron	Diltiazem hydrochloride	15B12-b01	1
Fagron	Diltiazem hydrochloride	15B12-B01-305401	3
Caelo	Diltiazem hydrochloride	1521806	1
Fagron	Diltiazem hydrochloride	15B12-B01-305299	1
Fagron	Diltiazem hydrochloride	14C12-B04-294135	1
Phönix	Diltiazem hydrochloride	15212801	1
Caelo	Diltiazem hydrochloride	15230503	9
Caelo	Diltiazem hydrochloride	15212806	2
Caelo	Diltiazem hydrochloride	15230501	3
Fagron	Diltiazem hydrochloride	15B12/B01305399	1
Fagron	Diltiazem hydrochloride	15b12-b01-305400	2
Caelo	Diltiazem hydrochloride	15230000000000000000	1
Caelo	Diltiazem hydrochloride	15B12-B01-305399	1
Phönix Gotha	Diltiazem hydrochloride	15230503	1
Caelo	Diltiazem hydrochloride	15230510	3
Caelo	Diltiazem hydrochloride	15230507	5
Fagron	Diltiazem hydrochloride	15G20-B08-310792	1
Caelo	Diltiazem hydrochloride	15230502	10
Fagron	Diltiazem hydrochloride	15G20-B08-312065	11
Caelo	Diltiazem hydrochloride	15G20-B08-312065	2
Caelo	Diltiazem hydrochloride	15230504	3
Chiesi/Phoenix	Diltiazem hydrochloride	15230502	1
Fagron	Diltiazem hydrochloride	15G20-B08	3
Fagron	Diltiazem hydrochloride	15G20-B08-314375	7
Fagron	Diltiazem hydrochloride	15G20-B02-310792	1
Fagron	Diltiazem hydrochloride	15B12-B01-305400	5
Caelo	Diltiazem hydrochloride	15230512	10
Fagron	Diltiazem hydrochloride	15B12B01305400	1
Caelo	Diltiazem hydrochloride	15414302	13
Fagron	Diltiazem hydrochloride	15g20-b08-314375	1
Caelo	Diltiazem hydrochloride	15G20-B08-314375	1
Caelo	Diltiazem hydrochloride	15230514	2
Fagron	Diltiazem hydrochloride	16A18-B07	5
Caelo	Diltiazem hydrochloride	15B12-B01-305400	1
Phoenix	Diltiazem hydrochloride	15230503	1
allianz	Diltiazem hydrochloride	15230512	1
Fagron	Diltiazem hydrochloride	16A18B07316667	1
Fagron	Diltiazem hydrochloride	16A18-B07-316667	6
Caesar&Loretz GmbH /Anzag	Diltiazem hydrochloride	15414302	1
Caelo	Diltiazem hydrochloride	16A18-B07-31667	1
Phönix	Diltiazem hydrochloride	15414302	1
Caelo	Diltiazem hydrochloride	15414301	13
Caelo	Diltiazem hydrochloride	15414305	2
Fagron	Diltiazem hydrochloride	16A18-B07-318732	13
Caelo	Diltiazem hydrochloride	15414309	2
Fagron	Diltiazem hydrochloride	DIL/M-10515	1
Fagron	Diltiazem hydrochloride	16C14-B11-320849	10
Nachprüfung	Diltiazem hydrochloride		1
Fagron	Diltiazem hydrochloride	16C14-B11-320568	4
Caelo	Diltiazem hydrochloride	15230515	1
Caelo	Diltiazem hydrochloride	16A18-B07-318732	2
Fagron	Diltiazem hydrochloride	16C14B11320849	1
Caelo	Diltiazem hydrochloride	15414313	11
Caelo	Diltiazem hydrochloride	140595	1
Caelo	Diltiazem hydrochloride	15230513	1
Caelo	Diltiazem hydrochloride	16A18-B07-318733	1
Fagron	Diltiazem hydrochloride	16a18-b07-318732	2
Jenne	Diltiazem hydrochloride	15414313	1

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Supplier	Substance	Batch	Spectra
Caelo	Diltiazem hydrochloride	261115DHC	1
Caelo	Diltiazem hydrochloride	160415D	1
Caelo	Diltiazem hydrochloride	15414321	2
Caelo	Diltiazem hydrochloride	15414319	15
Fagron	Diltiazem hydrochloride	16C14-B11-322642	14
Fagron	Diltiazem hydrochloride	16C14-B11-322153	6
Gehe	Diltiazem hydrochloride	15414319	1
Caelo	Diltiazem hydrochloride	15414318	1
Caelo	Diltiazem hydrochloride	16A18-B07-319570	1
ALH	Diltiazem hydrochloride	15414319	1
Fagron	Diltiazem hydrochloride	16A18-B07-319570	1
Caelo	Diltiazem hydrochloride	15230516	1
anzag	Diltiazem hydrochloride	15414319	2
Fagron	Diltiazem hydrochloride	16C14-B11-322152	5
Caelo	Diltiazem hydrochloride	15414303	1
Fagron	Diltiazem hydrochloride	15414313	1
Caelo	Diltiazem hydrochloride	154114319	1
Caelo	Diltiazem hydrochloride	16190806	10
Caesar & Loretz	Diltiazem hydrochloride	16190806	1
Fagron	Diltiazem hydrochloride	16C14-B11	3
Fagron	Diltiazem hydrochloride	16G20B03325903	1
Fagron	Diltiazem hydrochloride	16A18-B07-318733	3
Caelo	Diltiazem hydrochloride	16C14-B11-322153	2
Caelo	Diltiazem hydrochloride	15414320	1
Fagron	Diltiazem hydrochloride	16G20-B03	3
Caelo	Diltiazem hydrochloride	16190810	3
Fagron	Diltiazem hydrochloride	16G20-B03-328133	7
Fagron	Diltiazem hydrochloride	16G20-B03-325903	13
Caelo	Diltiazem hydrochloride	15414310	1
Caelo	Diltiazem hydrochloride	16190807	2
Caelo	Diltiazem hydrochloride	16190805	3
Fargon/Kehr	Diltiazem hydrochloride	16G20-B03-328133	1
Caelo	Diltiazem hydrochloride	15414312	1
Klosterring	Diltiazem hydrochloride	16190806	1
Sanacorp, 18.02.17, 16,...	Diltiazem hydrochloride	16190807	1
Caelo	Diltiazem hydrochloride	16G20-B03-328133	2
Caelo	Diltiazem hydrochloride	16190813	10
Caelo	Diltiazem hydrochloride	161908	1
phönix	Diltiazem hydrochloride	16G20-B03-328133	1
Sanacorp WE 17.02.17 E...	Diltiazem hydrochloride	16190806	1
Caelo	Diltiazem hydrochloride	16190801	1
Hedinger GmbH	Diltiazem hydrochloride	16G20-B03	1
Caelo	Diltiazem hydrochloride	15435807	1
Gehe	Diltiazem hydrochloride	16190813	1
Fagron	Diltiazem hydrochloride	16A14-B11-322153	1
Fagron	Diltiazem hydrochloride	16C14B11322152	1
Gehe	Diltiazem hydrochloride	16190806	1
Fagron	Diltiazem hydrochloride	16g20-b03-325903	1
Fagron	Diltiazem hydrochloride	16L19-B01-330365	7
Noweda	Diltiazem hydrochloride	15414319	1
Fagron	Diltiazem hydrochloride	DIL/M-21816	4
Caelo	Diltiazem hydrochloride	1250417	1
Caelo	Diltiazem hydrochloride	16L19-B01-330365	1
Caelo	Diltiazem hydrochloride	16190814	6
Caelo	Diltiazem hydrochloride	170602DH/16190813	1
Caelo	Diltiazem hydrochloride	1020617/16190813	1
Fagron	Diltiazem hydrochloride	17D11-B11-333704	9
Fagron	Diltiazem hydrochloride	16G20-B03-328253	2
GEHE	Diltiazem hydrochloride	16190813	1
Caelo	Diltiazem hydrochloride	17043202	9

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Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	16L19-B01-330396	4
Caelo	Diltiazem hydrochloride	17043205	3
Fagron	Diltiazem hydrochloride	AZ-0100716	1
Fagron	Diltiazem hydrochloride	16L19-B01	1
Noweda	Diltiazem hydrochloride	16L19-B01-330365	2
Caelo	Diltiazem hydrochloride	17043203	7
Fagron	Diltiazem hydrochloride	16GH20-B03-325903	1
Caelo	Diltiazem hydrochloride	170432	1
Caelo	Diltiazem hydrochloride	17043204	7
Caelo	Diltiazem hydrochloride	17043207	1
Fagron	Diltiazem hydrochloride	16c14-b11-322152	1
Anzag	Diltiazem hydrochloride	17043203	1
Caelo	Diltiazem hydrochloride	1090917/17043203	1
Caelo	Diltiazem hydrochloride	16190818	1
Caelo	Diltiazem hydrochloride	17043215	9
Fagron	Diltiazem hydrochloride	17D11-B11-334837	8
Caelo	Diltiazem hydrochloride	17043216	10
Fagron	Diltiazem hydrochloride	17043203	1
Fagron	Diltiazem hydrochloride	17D11-B11-334192	2
Fagron	Diltiazem hydrochloride	17D11-B11-333705	3
Caelo	Diltiazem hydrochloride	17D11-B11-333705	2
Bomastus / Alliance Hea...	Diltiazem hydrochloride	17043219	1
Phönix	Diltiazem hydrochloride	17d11-b11-334837	1
Caelo	Diltiazem hydrochloride	17043219	10
Fagron	Diltiazem hydrochloride	17D11-B11	3
Fagron	Diltiazem hydrochloride	16L19-B01330396	1
Caelo	Diltiazem hydrochloride	17043217	11
Caelo	Diltiazem hydrochloride	17043218	4
Fagron	Diltiazem hydrochloride	17H25-B01-340697	9
Fagron	Diltiazem hydrochloride	16L19-B01-330395	1
p&m cosmetics/gehe	Diltiazem hydrochloride	17043217	1
Caelo	Diltiazem hydrochloride	17043212	1
Fagron	Diltiazem hydrochloride	17H25-B01-340699	1
Fagron	Diltiazem hydrochloride	AZ-0641216	1
Caelo	Diltiazem hydrochloride	17043228	4
Fagron	Diltiazem hydrochloride	17H25-B01-340697	1
Fagron	Diltiazem hydrochloride	17D11-B11-336727	1
Fagron	Diltiazem hydrochloride	17H25-B01-341597	2
Sanacorp	Diltiazem hydrochloride	17043217	1
Fagron	Diltiazem hydrochloride	17H25-B01	2
Caelo	Diltiazem hydrochloride	17043224	2
AHD	Diltiazem hydrochloride	17043210	1
Caelo	Diltiazem hydrochloride	180320DHC/17043218	1
Fagron	Diltiazem hydrochloride	17H25-B01-341596	4
Caelo	Diltiazem hydrochloride	17H25-B01-340697	1
GEHE	Diltiazem hydrochloride	17043217	1
Caelo	Diltiazem hydrochloride	17337007	2
Caesar & Lorenz GmbH	Diltiazem hydrochloride	17043218	1
Kehr	Diltiazem hydrochloride	17043228	1
Fagron	Diltiazem hydrochloride	17H25-B01-343273	3
Caelo	Diltiazem hydrochloride	17H25-B01-343273	1
Sanacorp	Diltiazem hydrochloride	17337005	1
Caelo	Diltiazem hydrochloride	17043230	2
Fragon/Noweda	Diltiazem hydrochloride	16L19-B01-330396	1
Fagron	Diltiazem hydrochloride	18A29-B01	1
Caelo	Diltiazem hydrochloride	17337005	8
Fagron	Diltiazem hydrochloride	18A29-B01-345623	2
Caeolo	Diltiazem hydrochloride	17337005	2
Caelo	Diltiazem hydrochloride	17337012	6
Caelo	Diltiazem hydrochloride	17337010	4

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Supplier	Substance	Batch	Spectra
Caelo	Diltiazem hydrochloride	1733712	1
Fagron	Diltiazem hydrochloride	18A29-B01-346695	2
Gehe	Diltiazem hydrochloride	17337005	1
Caelo	Diltiazem hydrochloride	17332021	1
Fiebig	Diltiazem hydrochloride	17043227	1
Fagron	Diltiazem hydrochloride	18A29-B01-347886	5
Fagron	Diltiazem hydrochloride	18A29-B01-346694	2
Caelo	Diltiazem hydrochloride	17337009	9
Fagron	Diltiazem hydrochloride	18A29-01-347886	1
Caelo	Diltiazem hydrochloride	17337004	3
Caelo	Diltiazem hydrochloride	17043213	1
Fagron	Diltiazem hydrochloride	18A29-B01-348861	6
Fagron	Diltiazem hydrochloride	18A29-B01-350964	1
Caelo	Diltiazem hydrochloride	18H09-B03-352908	1
Caelo	Diltiazem hydrochloride	17337018	3
Gehe	Diltiazem hydrochloride	17337026	1
Fagron	Diltiazem hydrochloride	18A29-B01-345623	1
Caelo	Diltiazem hydrochloride	17337026	3
Caelo	Diltiazem hydrochloride	17337014	2
Caelo	Diltiazem hydrochloride	1733701	1
Fagron	Diltiazem hydrochloride	18A29-B01-352909	1
Caelo	Diltiazem hydrochloride	17337027	1
Caelo	Diltiazem hydrochloride	18301111	1

- 77 802 spectra from 565 *Apo-Ident* customers from a total of 25 855 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Diltiazem hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diltiazem hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	280	0	126 612
Type C	0	1003	124	77 802

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.8817 %)	88.9973 % (> 88.7311 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
23016	22631	16.88	54.11
21270	22631	13.43	49.74
21300	22631	5.89	44.44
22631	22631	0.00	48.94

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Dimethyl fumarate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21558-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dimethyl fumarate

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 fumarate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dimethyl fumarate	13269801	21558	40	1506634
Euro OTC	Dimethyl fumarate	1410013-01	21833	40	20141125

Validation samples

A total of 280 317 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 fumarate*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Dimethyl fumarate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dimethyl fumarate	13269801	21558 [†]	20
Euro OTC	Dimethyl fumarate	1410013-01	21833 [†]	20
Euro OTC	Dimethyl fumarate	1601013-01	23907	40

- 126 812 spectra from a total of 2786 batches from further 781 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 fumarate*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were 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 fumarate* can clearly be 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 fumarate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	80	0	126 812
Type C	0	0	0	78 929

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8817 %)	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
21558	21558	0.00	64.42
21833	21558	7.26	71.39

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Diphenhydramine hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20186-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Diphenhydramine hydrochloride; Diphenhydramini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Diphenhydramine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Diphenhydramine ...	12329816	21464	30	20121119
Caelo	Diphenhydramine ...	16004901	23235	40	20160122
Fagron	Diphenhydramine ...	16C25-B03-331026	23262	40	AR-17-FG-015432-02

Validation samples

A total of 280317 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 *Diphenhydramine - hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74386 spectra from a total of 1620 batches from further 372 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 5 reference samples from the substance/substance group *Diphenhydramine - hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Diphenhydramine hydrochloride	12329816	21304	40
Caelo	Diphenhydramine hydrochloride	12329816	21464 [†]	30
Caelo	Diphenhydramine hydrochloride	15072617	23206	40
Caelo	Diphenhydramine hydrochloride	172276	23803	40
Caelo	Diphenhydramine hydrochloride	183010	24390	40

- 126702 spectra from a total of 2785 batches from further 781 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.

- 74 spectra from 48 *Apo-Ident* customers from 44 batches from the substance/substance group *Diphenhydramine hydrochloride*.

[†]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
Finze	Diphenhydramine hydrochloride	9F05-N04	2
Caelo	Diphenhydramine hydrochloride	10122030	1
Caelo	Diphenhydramine hydrochloride	5121204	1
Fagron	Diphenhydramine hydrochloride	12F28-N01	1
Fagron	Diphenhydramine hydrochloride	12J04-N02	1
Caelo	Diphenhydramine hydrochloride	12007702	1
Caelo	Diphenhydramine hydrochloride	25071306	1
Caelo	Diphenhydramine hydrochloride	12007716	1
Noweda	Diphenhydramine hydrochloride	12007716	1
Caelo	Diphenhydramine hydrochloride	12007713	2
Caelo	Diphenhydramine hydrochloride	12007721	2
Caelo	Diphenhydramine hydrochloride	12007715	2
Caesar/Noweda	Diphenhydramine hydrochloride	12007714	1
Sanacorp	Diphenhydramine hydrochloride	12329805	1
Caelo	Diphenhydramine hydrochloride	2041403	1
Caelo	Diphenhydramine hydrochloride	1912I-01339	1
PHOENIX 29.01.2013	Diphenhydramine hydrochloride	120208	1
Caelo	Diphenhydramine hydrochloride	12329815	2
Fagron	Diphenhydramine hydrochloride	13A14-B40-293346	1
Caelo	Diphenhydramine hydrochloride	13343104	1
Caelo	Diphenhydramine hydrochloride	31031508	1
Caelo	Diphenhydramine hydrochloride	1814A-01339	1
Caelo	Diphenhydramine hydrochloride	13331810	1
Gatt-Koller	Diphenhydramine hydrochloride	606030315	1
Caelo	Diphenhydramine hydrochloride	15072602	3
Caelo	Diphenhydramine hydrochloride	20071502	1
Caelo	Diphenhydramine hydrochloride	13331813	1
Caelo	Diphenhydramine hydrochloride	15072630	1
Caelo	Diphenhydramine hydrochloride	12329805	1
Caelo	Diphenhydramine hydrochloride	15072603	4
Caelo	Diphenhydramine hydrochloride	15220402	1
Caelo	Diphenhydramine hydrochloride	15220403	3
Noweda	Diphenhydramine hydrochloride	15220402	1
Caelo	Diphenhydramine hydrochloride	15220404	3
Caelo	Diphenhydramine hydrochloride	2215I-01339	1
Caelo	Diphenhydramine hydrochloride	15220405	2
Caelo	Diphenhydramine hydrochloride	15072608	1
Caelo	Diphenhydramine hydrochloride	15072609	4
Caelo	Diphenhydramine hydrochloride	13100462	1
Caelo	Diphenhydramine hydrochloride	15072614	5
Caelo	Diphenhydramine hydrochloride	3071715	1
Sanacorp	Diphenhydramine hydrochloride	15072617	1
Phönix WE: 07.01.14 EK...	Diphenhydramine hydrochloride	12329805	1
Fagron	Diphenhydramine hydrochloride	16C25-B03-331026	1
Caelo	Diphenhydramine hydrochloride	16004908	2
Caelo	Diphenhydramine hydrochloride	15072617	1
Caelo	Diphenhydramine hydrochloride	16004910	2
Caelo	Diphenhydramine hydrochloride	18008201	2
Caelo	Diphenhydramine hydrochloride	18008205	1

- 78 855 spectra from 565 *Apo-Ident* customers from a total of 26 094 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Diphenhydramine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diphenhydramine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 386
Type B	0	190	0	126 702
Type C	0	49	25	78 855

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 94.5455 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.8817 %)	66.2162 % (> 62.1622 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21464	23262	8.74	33.04
23235	23262	9.01	33.64
23262	23262	0.00	28.92

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Diphenylcyclopropenone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20934-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Diphenylcyclopropenone; Diphenylcyclopropenonum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Diphenylcyclopropenone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Diphenylcyclopro...	12L17-N07	20934	40	1407599
Fagron	Diphenylcyclopro...	15J12-B01-316620	22362	40	9341
Fagron	Diphenylcyclopro...	16F02-B10-329708	23070	40	1902476

Validation samples

A total of 280317 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 *Diphenylcyclopropanone*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 [†].

- 135 spectra of 4 reference samples from the substance/substance group *Diphenylcyclopropanone*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Diphenylcyclopropanone	13I26-N12	21342	40
Fagron	Diphenylcyclopropanone	13I26-N12	21539	35
Fagron	Diphenylcyclopropanone	15J12-B01-316620	22362 [†]	20
Fagron	Diphenylcyclopropanone	16F02-B10-326265	23071	40

- 126757 spectra from a total of 2786 batches from further 781 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 4 batches from the substance/substance group *Diphenylcyclopropanone*.

Supplier	Substance	Batch	Spectra
Fagron	Diphenylcyclopropanone	16F02-B10-327812	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*.

continued from previous page

Supplier	Substance	Batch	Spectra
Frago/Noweda	Diphenylcyclopropenone	16F02-B10-324263	2
Fagron	Diphenylcyclopropenone	35-16-I-95P3117	1
Euro OTC	Diphenylcyclopropenone	17B-13B02-334769	1

- 78 923 spectra from 565 *Apo-Ident* customers from a total of 26 133 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Diphenylcyclopropenone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diphenylcyclopropenone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	20	115	126 757
Type C	0	6	0	78 923

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	14.8148 % (> 12.5926 %)
Type C	100.0000 % (> 99.8819 %)	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
20934	20934	0.00	31.57
23070	23070	0.00	23.40
22362	22362	0.00	22.97

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Dithranol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20032-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dithranol; Dithranolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Dithranol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Dithranol	1702022-01	24153	40	1809448
Caelo	Dithranol	18115302	24169	40	1811302
Fagron	Dithranol	18B23-B05-348137	24172	40	20180430
Caelo	Dithranol	18190604	24429	40	1904372

Validation samples

A total of 280 317 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 *Dithranol*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Dithranol*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Dithranol	1203025-02	20873	40
Audor Pharma	Dithranol	APOP_DNL711/17/001D	24173	40

- 126 812 spectra from a total of 2787 batches from further 781 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.

- 83 spectra from 60 *Apo-Ident* customers from 41 batches from the substance/substance group *Dithranol*.

Supplier	Substance	Batch	Spectra
Euro OTC	Dithranol		1
Caelo	Dithranol	11064501	1
Euro OTC	Dithranol	1008011-02	2

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Supplier	Substance	Batch	Spectra
Caelo	Dithranol	12014504	2
Audor Pharma	Dithranol	APDT/365/2011	2
Audor Pharma	Dithranol	APDT/365/2011D	1
Caelo	Dithranol		1
Euro OTC	Dithranol	1008011-01	1
Caelo	Dithranol	APDT/3652011D	1
Audor Pharma	Dithranol	APDT/351/2010D	1
Fagron	Dithranol	17710I-01274	1
Caelo	Dithranol	27111206	1
Euro OTC	Dithranol	1203025-02	14
Caelo	Dithranol	12014502	1
Caelo	Dithranol	12236811	4
Noweda	Dithranol	APDT/375/2012	1
Noweda	Dithranol	1203025-02	1
Sanacorp	Dithranol	APDT/375/2012	1
Caelo	Dithranol	12236809	1
EuRho	Dithranol	1203025-01	1
Gehe/Audar	Dithranol	APDT3752012D	1
Audor Pharma	Dithranol	APDT/375/2012D	8
Caelo	Dithranol	APDT/375/2012D	3
Caelo	Dithranol	12375302	4
Audor Pharma	Dithranol	DT/375/2012D	2
Noweda	Dithranol	DT/375/2012D	1
Caelo	Dithranol	12375403	1
Audor Pharma	Dithranol	APDT3752012D	1
Fagron	Dithranol	13A30-N01	4
Caelo	Dithranol	12375601	1
Caelo	Dithranol	12375305	1
Anzag	Dithranol	120302502	1
Fagron	Dithranol	11L20-N13	1
Caelo	Dithranol	1212I-01274	1
Caelo	Dithranol	1203025-02	1
Caelo	Dithranol	13120503	1
Euro OTC	Dithranol	56/11072013	1
Euro OTC	Dithranol	DT/370/2012	1
Audor Pharma	Dithranol	DT/351/2010D	1
Caelo	Dithranol	13120504	1
Caelo	Dithranol	13120502	1
Caelo	Dithranol	13120702	1
Gehe	Dithranol	1311029-01	1
Caelo	Dithranol	14101715	1
Euro OTC	Dithranol	1311029-01	1
Audor Pharma	Dithranol	APDT3902013D	1
Audor Pharma	Dithranol	APOP-DNL/11/17/001	1
Sanacorp	Dithranol	APOP-DNL/11/17/001-D	1

- 78 846 spectra from 565 *Apo-Ident* customers from a total of 26 096 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

relevant spectra of the various substances were compared with *Dithranol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	55	25	126 812
Type C	0	32	51	78 846

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	68.7500 % (> 65.0000 %)
Type C	100.0000 % (> 99.8817 %)	38.5542 % (> 34.9398 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
24153	24153	0.00	40.99
24429	24429	0.00	48.63
24169	24169	0.00	77.11
24172	24169	3.93	76.02

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Doxycycline hyclate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20796-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Doxycycline hyclate; Doxycyclini hyclas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Doxycycline hyclate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Doxycycline hycl...	12G12-N15	20796	40	1404233
Fagron	Doxycycline hycl...	12G12-N15	20821	40	20120807
Fagron	Doxycycline hycl...	14K28-B05-312218	22242	40	20150216

Validation samples

A total of 280 317 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 *Doxycycline hyclate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1621 batches from further 372 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 *Doxycycline hyclate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Doxycycline hyclate	14K28-B05-312218	22242 [†]	20
Fagron	Doxycycline hyclate	16I06-B02-330167	23118	40
Fagron	Doxycycline hyclate	18D18-B01-349567	24170	40

- 126 792 spectra from a total of 2786 batches from further 781 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 8 *Apo-Ident* customers from 15 batches from the substance/substance group *Doxycycline hyclate*.

Supplier	Substance	Batch	Spectra
Löwen City-Apotheke Bar...	Doxycycline hyclate	10022014	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	Doxycycline hyclate	12G12-N15	1
Löwen City-Apotheke Bar...	Doxycycline hyclate	2042015	1
Fagron	Doxycycline hyclate	14K28-B05-312010	1
Fagron	Doxycycline hyclate	13D24-B40-298948	1
Fagron	Doxycycline hyclate	16I06-B02-330167	1
Fagron	Doxycycline hyclate	16E04-B07-231917	1
Fagron	Doxycycline hyclate	20101701	1
Fagron	Doxycycline hyclate	16106-Bo2	1
Fagron	Doxycycline hyclate	1603008	1
Fagron	Doxycycline hyclate	16I06-B02-330167	1
Fagron	Doxycycline hyclate	16I06-B02	1
Sanacorp	Doxycycline hyclate	16I06-B02-335675	1
Fagron	Doxycycline hyclate	17112201	1
Caelo	Doxycycline hyclate	16I06-B02-341857	1

- 78 914 spectra from 565 *Apo-Ident* customers from a total of 26 123 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Doxycycline hyclate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Doxycycline hyclate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	78	22	126 792
Type C	0	14	1	78 914

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	78.0000 % (> 75.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
22242	20796	11.56	25.96
20796	20796	0.00	24.70
20821	20796	2.14	24.34

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Doxylamine hydrogen succinate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20315-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Doxylamine hydrogen succinate; Doxylamine succinate; Doxylamini hydrogenosuccinas

Special notes

When selecting the *Doxylamine hydrogen succinate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Doxylamine hydrogen succinate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Doxylamine hydro...	14F03-B01-293498	21542	40	1410524
Fagron	Doxylamine hydro...	15F01-B04-309189	22601	40	AR-16-FG-011361-01
Caelo	Doxylamine hydro...	15203906	23085	40	20151112

Validation samples

A total of 280 317 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 *Doxylamine hydrogen succinate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Doxylamine hydrogen succinate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Doxylamine hydrogen succinate	14F03-B01-293498	21542 [†]	20
Caelo	Doxylamine hydrogen succinate	15203906	23086	40
Caelo	Doxylamine hydrogen succinate	172047	23626	40

- 126 792 spectra from a total of 2786 batches from further 781 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 16 *Apo-Ident* customers from 24 batches from the substance/substance group *Doxylamine hydrogen succinate*.

Supplier	Substance	Batch	Spectra
Fagron	Doxylamine hydrogen succinate	12E04-N04	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
Fagron	Doxylamine hydrogen succinate	11K17-N04	3
Fagron	Doxylamine hydrogen succinate	11G20-N10	1
Fagron	Doxylamine hydrogen succinate	12G10-N03	6
Caesar & Loretz GmbH, 4...	Doxylamine hydrogen succinate	13A04-N02	4
Fagron	Doxylamine hydrogen succinate	13A04-N02	3
Fagron	Doxylamine hydrogen succinate	12K21-N01	2
Fagron	Doxylamine hydrogen succinate	13E29-N03	4
Fagron	Doxylamine hydrogen succinate	13/26-N14	1
Fagron	Doxylamine hydrogen succinate	12811328003	1
Fagron	Doxylamine hydrogen succinate	12811420001	1
Fagron	Doxylamine hydrogen succinate	14F03-B01-296845	1
Fagron	Doxylamine hydrogen succinate	14K27-B07-303356	1
Fagron	Doxylamine hydrogen succinate	15F01-B04-308354	1
Caelo	Doxylamine hydrogen succinate	14k27-B07	1
Fagron	Doxylamine hydrogen succinate	15F01-B04-309189	3
Fagron	Doxylamine hydrogen succinate	14F03B01293498	1
Fagron	Doxylamine hydrogen succinate	483875887	1
Fagron	Doxylamine hydrogen succinate	14K27-B07	1
Caelo	Doxylamine hydrogen succinate	15F01-B04-317385	2
Fagron	Doxylamine hydrogen succinate	15K04-B01	1
Caelo	Doxylamine hydrogen succinate	15K04B01327356	1
Fagron	Doxylamine hydrogen succinate	15K04-B01-327356	1
Fagron	Doxylamine hydrogen succinate	18041818	1
Fagron	Doxylamine hydrogen succinate	16F06-B-02-338804	1

- 78 883 spectra from 565 *Apo-Ident* customers from a total of 26 113 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Doxylamine hydrogen succinate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Doxylamine hydrogen succinate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	39	7	78 883

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	84.7826 % (> 78.2609 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
23085	22601	7.55	36.31
22601	22601	0.00	31.35
21542	21542	0.00	36.17

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Drofenine hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20320-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Drofenine hydrochloride; Drofenini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Drofenine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Drofenine hydroc...	13I09-N05	21275	40	20130524
Fagron	Drofenine hydroc...	15G01-B04-330979	23233	40	AR-17-FG-015434-02

Validation samples

A total of 280 317 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 *Drofenine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Drofenine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Drofenine hydrochloride	15G01-B04-323028	22807	40
Fagron	Drofenine hydrochloride	15G01-B04-330979	23412	40
Fagron	Drofenine hydrochloride	18A18-B99-345993	24106	40

- 126 772 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Drofenine hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	Drofenine hydrochloride	11J24-N01	1
Fagron	Drofenine hydrochloride	12D04-N03	1

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Drofenine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Drofenine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	120	0	126 772
Type C	0	2	0	78 927

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8823 %)	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
21275	23233	6.16	48.88
23233	23233	0.00	49.89

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Eosin Y**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20571-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Eosin Y; Eosinum natricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Eosin Y*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Eosin Y	12E25-N01	20900	55	20120607
Fagron	Eosin Y	15G01-T03-025958	22261	40	1604114
Fagron	Eosin Y	13F14-T01-017395	22534	40	1608469
Fagron	Eosin Y	13F14-T01-017395	22660	40	1801115
Fagron	Eosin Y	13F14-T01-017395	22816	40	1705197
Fagron	Eosin Y	17K21-T07-042542	23975	40	1805338

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 255 spectra of 6 reference samples from the substance/substance group *Eosin Y*. These samples are listed above in the [calibration samples](#) section.
- 74241 spectra from a total of 1619 batches from further 372 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 [†].

- 145 spectra of 5 reference samples from the substance/substance group *Eosin Y*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Eosin Y	12E25-N01	20900 [†]	5
Fagron	Eosin Y	13I11-N03	20932	40
Fagron	Eosin Y	13I11-N03	21208	40
Fagron	Eosin Y	15G01-T03-025958	22261 [†]	20
Fagron	Eosin Y	13F14-T01-017395	22535	40

- 126747 spectra from a total of 2785 batches from further 781 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.

- 47 spectra from 41 *Apo-Ident* customers from 24 batches from the substance/substance group *Eosin Y*.

[†]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	Eosin Y	12e25-n01	1
Fagron	Eosin Y	11E25-N01	1
Fagron	Eosin Y	12A02-N09	2
Sanacorp	Eosin Y	12E25-N01	1
Fagron	Eosin Y	11F21-N10	1
Fagron	Eosin Y	12E25-N01	4
Fagron	Eosin Y	12H28-N08	2
Fagron	Eosin Y	EYWS/16/11	2
Caelo	Eosin Y	12e25n01	1
Fargon/Sanacorp	Eosin Y	13/11-No3	1
Fagron	Eosin Y	13/11-N03	1
Fagron	Eosin Y	13/11-N03	3
Caelo	Eosin Y	13I11-N03	1
Caelo	Eosin Y	14H28-M05	1
Fagron	Eosin Y	EYWS/15/13	1
Fagron	Eosin Y	14H28-M09	2
sanacorp	Eosin Y	14H28-M05	1
Gehe	Eosin Y	14H28-M05	1
Caelo	Eosin Y	13F14-T01-017395	1
Fagron	Eosin Y	13F14-T01-017395	5
Fagron	Eosin Y	14H28-M05	2
Cael Sanacorp 05.02.2016	Eosin Y	13F14-T01-017395	1
Fagron	Eosin Y	15G01T03025959	1
Fagron	Eosin Y	15G01-T03-025958	2
Fagron	Eosin Y	13fF14-T01-017395	1
Fagron	Eosin Y	17372-87-1	1
Fagron	Eosin Y	15G01-T03-027933	2
Fagron	Eosin Y	15G01-T03-034438	1
Caelo	Eosin Y	15G01-T03-025958	1
Fagron	Eosin Y	17K21-T07-042542	1
Fagron	Eosin Y	17K21T07-054710	1

- 78 882 spectra from 565 *Apo-Ident* customers from a total of 26 113 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	255	0	74 241
Type B	0	134	11	126 747
Type C	0	20	27	78 882

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.6471 %)
Type B	100.0000 % (> 99.9901 %)	92.4138 % (> 90.3448 %)
Type C	100.0000 % (> 99.8817 %)	42.5532 % (> 36.1702 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22534	22534	0.00	62.26
22261	22261	0.00	53.95
22660	22660	0.00	71.84
20900	23975	16.59	66.76
23975	23975	0.00	72.63
22816	22816	0.00	72.03

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Ephedrine hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20993-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ephedrine hydrochloride; Ephedrini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Ephedrine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ephedrine hydroc...	12017217	20993	40	1511635
Caelo	Ephedrine hydroc...	13323305	21322	40	20131113
Caelo	Ephedrine hydroc...	14378502	21803	40	20150106
Caelo	Ephedrine hydroc...	161197	22436	40	20160420*
Fagron	Ephedrine hydroc...	17G05-B05-337987	23927	40	20170901

Validation samples

A total of 280 317 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 *Ephedrine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1618 batches from further 372 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 *Ephedrine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ephedrine hydrochloride	14378502	21803 [†]	20
Caelo	Ephedrine hydrochloride	161197	22436 [†]	20
Fagron	Ephedrine hydrochloride	15H28-B02-316349	23073	40
Caelo	Ephedrine hydrochloride	171736	23672	40

- 126 772 spectra from a total of 2785 batches from further 781 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*.

- 41 spectra from 20 *Apo-Ident* customers from 35 batches from the substance/substance group *Ephedrine hydrochloride*.

Supplier	Substance	Batch	Spectra
Caelo	Ephedrine hydrochloride	11126407	1
Caelo	Ephedrine hydrochloride	10103425	1
Caelo	Ephedrine hydrochloride	12017209	2
Caesar & Loretz GmbH, 4...	Ephedrine hydrochloride	11126411	1
Fagron	Ephedrine hydrochloride	12017220	1
Fagron	Ephedrine hydrochloride	13B19-N04	1
Caelo	Ephedrine hydrochloride	12017215	1
Caelo	Ephedrine hydrochloride	12017217	1
Caelo	Ephedrine hydrochloride	12017223	1
Caelo	Ephedrine hydrochloride	13323302	1
Phoenix 04.03.14	Ephedrine hydrochloride	1332303	1
Gehe am 04.03.14	Ephedrine hydrochloride	13323303	1
PHOENIX 10.03.2014	Ephedrine hydrochloride	13323302	1
Fagron	Ephedrine hydrochloride	13L30-B36	1
Gatt-Koller / Phoenix	Ephedrine hydrochloride	18502141114	1
Caelo	Ephedrine hydrochloride	13323305	2
GATT-KOLLER/PHOENIX	Ephedrine hydrochloride	915/03141314	2
Caelo	Ephedrine hydrochloride	13323310	1
Phönix	Ephedrine hydrochloride	13323315	1
Caelo	Ephedrine hydrochloride	13323316	1
Caelo	Ephedrine hydrochloride	14378502	1
Caelo	Ephedrine hydrochloride	14378506	2
Caelo	Ephedrine hydrochloride	14378510	1
Caelo	Ephedrine hydrochloride	151J9304	1
Caelo	Ephedrine hydrochloride	14378507	1
Caesar & Loretz GmbH	Ephedrine hydrochloride	14378503	1
Caelo	Ephedrine hydrochloride	16119703	1
Caelo	Ephedrine hydrochloride	15179302	1
Caelo	Ephedrine hydrochloride	16119702	1
Caelo	Ephedrine hydrochloride	1619704	1
Caelo	Ephedrine hydrochloride	16119709	1
Caelo	Ephedrine hydrochloride	10119709	1
Caelo	Ephedrine hydrochloride	16119715200218P301	1
Caelo	Ephedrine hydrochloride	18006701	1
Caelo	Ephedrine hydrochloride	16119715	2
Caelo	Ephedrine hydrochloride	18006709	1

- 78 888 spectra from 565 *Apo-Ident* customers from a total of 26 102 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ephedrine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ephedrine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	120	0	126 772
Type C	0	41	0	78 888

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 85.3659 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
23927	22436	27.45	55.38
20993	20993	0.00	40.29
21322	20993	3.47	39.79
21803	22436	4.15	41.92
22436	22436	0.00	43.16

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Epinephrine hydrogen tartrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20689-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Epinephrine hydrogen tartrate; Adrenaline hydrogen tartrate; Adrenalini tartras

Special notes

When selecting the *Epinephrine hydrogen tartrate* substance/substance group, the following information is displayed to the user:

- Advice for the identification of epinephrine bitartrate: According to the BfArM, ephedrine and its salts are considered as critical drugs in compliance to § 5 AMG. Critical drugs must not be placed on the market or be applied to humans.

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Epinephrine hydrogen tartrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Epinephrine hydr...	12120202	20689	40	1405614
Fagron	Epinephrine hydr...	12L22-N04	20749	40	20120106
Caelo	Epinephrine hydr...	12337804	21058	40	20121128

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Epinephrine hydr...	14007802	21489	40	1603180
Caelo	Epinephrine hydr...	14007802	21490	40	20140130
Caelo	Epinephrine hydr...	14007802	21489SI	40	1603180

Validation samples

A total of 280317 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 *Epinephrine hydrogen tartrate*. These samples are listed above in the [calibration samples](#) section.
- 74256 spectra from a total of 1619 batches from further 372 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 [†].

- 820 spectra of 28 reference samples from the substance/substance group *Epinephrine hydrogen tartrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Epinephrine hydrogen tartrate	12337805	21059	40
Caelo	Epinephrine hydrogen tartrate	14007802	21489 [†]	20
Caelo	Epinephrine hydrogen tartrate	14007802	21490 [†]	20
Caelo	Epinephrine hydrogen tartrate	14007802	21491	20
Caelo	Epinephrine hydrogen tartrate	14007802	21492	20
Caelo	Epinephrine hydrogen tartrate	14007802	21493	20
Caelo	Epinephrine hydrogen tartrate	14007802	21494	60
Caelo	Epinephrine hydrogen tartrate	14007802	21495	20
Caelo	Epinephrine hydrogen tartrate	14007802	21496	20
Caelo	Epinephrine hydrogen tartrate	14007802	21497	20
Caelo	Epinephrine hydrogen tartrate	14007802	21498	20
Caelo	Epinephrine hydrogen tartrate	162764	22777	40
Caelo	Epinephrine hydrogen tartrate	171115	23323	40
Caelo	Epinephrine hydrogen tartrate	171115	23326	40
Caelo	Epinephrine hydrogen tartrate	181795	24260	40
Caelo	Epinephrine hydrogen tartrate	14007802	21489SI [†]	20
Caelo	Epinephrine hydrogen tartrate	14007802	21490SI	60
Caelo	Epinephrine hydrogen tartrate	14007802	21491SI	20
Caelo	Epinephrine hydrogen tartrate	14007802	21492SI	20
Caelo	Epinephrine hydrogen tartrate	14007802	21493SI	20

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Epinephrine hydrogen tartrate	14007802	21495SI	20
Caelo	Epinephrine hydrogen tartrate	14007802	21496SI	20
Caelo	Epinephrine hydrogen tartrate	14007802	21497SI	20
Caelo	Epinephrine hydrogen tartrate	14007802	21498SI	20
Caelo	Epinephrine hydrogen tartrate	162764	22777SI	40
Caelo	Epinephrine hydrogen tartrate	171115	23323SI	40
Caelo	Epinephrine hydrogen tartrate	171115	23326SI	40
Caelo	Epinephrine hydrogen tartrate	181795	24260SI	40

- 126 072 spectra from a total of 2784 batches from further 781 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 21 *Apo-Ident* customers from 28 batches from the substance/substance group *Epinephrine hydrogen tartrate*.

Supplier	Substance	Batch	Spectra
Caelo	Epinephrine hydrogen tartrate	10237109	1
Caelo	Epinephrine hydrogen tartrate	12120202	1
Fagron	Epinephrine hydrogen tartrate	12G11-N07	1
Fagron	Epinephrine hydrogen tartrate	12G11-No70076/130	1
Caelo	Epinephrine hydrogen tartrate	12337805	2
Fagron	Epinephrine hydrogen tartrate	13I04-N03	1
Fagron	Epinephrine hydrogen tartrate	12/02-N03	1
Caelo	Epinephrine hydrogen tartrate	12337801	1
Caelo	Epinephrine hydrogen tartrate	123337805	1
Alliance Health 12.03.14	Epinephrine hydrogen tartrate	12337805	1
Fagron	Epinephrine hydrogen tartrate	13I04-N03	1
Phoenix 22.5.14	Epinephrine hydrogen tartrate	12337804	1
AHD 17.11.14 EK 7,60	Epinephrine hydrogen tartrate		1
Caelo	Epinephrine hydrogen tartrate	14007808	1
Fagron	Epinephrine hydrogen tartrate	14E12-B02	1
Caelo	Epinephrine hydrogen tartrate	14301002	2
Caelo	Epinephrine hydrogen tartrate	15239701	2
Fagron	Epinephrine hydrogen tartrate	15A13-B02-305559	2
Caelo	Epinephrine hydrogen tartrate	15239703	1
Caelo	Epinephrine hydrogen tartrate	15194102	1
Caelo	Epinephrine hydrogen tartrate	210316-1	1
Caelo	Epinephrine hydrogen tartrate	210316-3	1
Fagron	Epinephrine hydrogen tartrate	16E09-B11-319882	4
Caelo	Epinephrine hydrogen tartrate	15194104	1
Fagron	Epinephrine hydrogen tartrate	16e09-b11-319882	1
Caelo	Epinephrine hydrogen tartrate	16276402	1
Caelo	Epinephrine hydrogen tartrate	162746402	1
Caelo	Epinephrine hydrogen tartrate	17111503	2
Fagron	Epinephrine hydrogen tartrate	12011902	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*.

- 78 892 spectra from 565 *Apo-Ident* customers from a total of 26 109 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Epinephrine hydrogen tartrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Epinephrine hydrogen tartrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	814	6	126 072
Type C	0	37	0	78 892

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	99.2683 % (> 98.9024 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 83.7838 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20689	20689	0.00	55.58
20749	21489	11.95	55.37
21058	20689	2.98	55.04
21489	21489	0.00	57.72
21490	21489	14.92	63.10

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ergotamine tartrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21341-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ergotamine tartrate; Ergotamini tartras

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ergotamine tartrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ergotamine tartr...	15B16-B05-308418	22361	30	9384
Fagron	Ergotamine tartr...	15B16-B05-308417	22722	40	20150302
Fagron	Ergotamine tartr...	15B16-B05-308418	22361SI	30	9384
Fagron	Ergotamine tartr...	15B16-B05-308417	22722SI	40	20150302

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 4 reference samples from the substance/substance group *Ergotamine tartrate*. These samples are listed above in the [calibration samples](#) section.
- 74 356 spectra from a total of 1621 batches from further 372 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 5 reference samples from the substance/substance group *Ergotamine tartrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ergotamine tartrate	13H02-N01	21341	100
Fagron	Ergotamine tartrate	13I24-B10-288648	21540	50
Fagron	Ergotamine tartrate	13I24-B10-288650	21556	60
Fagron	Ergotamine tartrate	15B16-B05-308418	22361 [†]	15
Fagron	Ergotamine tartrate	15B16-B05-308418	22361SI [†]	15

- 126 652 spectra from a total of 2785 batches from further 781 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 *Ergotamine tartrate*.

[†]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*.

- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ergotamine tartrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ergotamine tartrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 356
Type B	0	79	161	126 652
Type C	0	0	0	78 929

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9901 %)	32.9167 % (> 31.6667 %)
Type C	100.0000 % (> 99.8817 %)	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
22722	22361	13.37	56.88
22361	22361	0.00	41.16

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Erythromycin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20011-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Erythromycin; Erythromycinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Erythromycin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Erythromycin	12E24-N04	21056	60	20120607
Caelo	Erythromycin	13175601	21323	40	20130620
Euro OTC	Erythromycin	1308016-02	21651	40	1412542
Fagron	Erythromycin	14B06-B35-290872	21669	40	20140225
Euro OTC	Erythromycin	1508034	21890	40	20150925*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Erythromycin	160792	22438	40	20160408*
Euro OTC	Erythromycin	1607038	22832	40	20160831*
Euro OTC	Erythromycin	1705038	23438	40	20170705*
Euro OTC	Erythromycin	1811019	24420	40	20190114*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 380 spectra of 9 reference samples from the substance/substance group *Erythromycin*. These samples are listed above in the [calibration samples](#) section.
- 74116 spectra from a total of 1614 batches from further 372 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 [†].

- 408 spectra of 10 reference samples from the substance/substance group *Erythromycin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Erythromycin	1308016-02	21651 [†]	20
Fagron	Erythromycin	14B06-B35-290872	21669 [†]	20
Euro OTC	Erythromycin	1508034	21890 [†]	20
Caelo	Erythromycin	160792	22438 [†]	20
Caelo	Erythromycin	160795	22439	60
Caelo	Erythromycin	160797	22440	60
Caelo	Erythromycin	160796	22442	60
Caelo	Erythromycin	13175601	21323SI	48
Fagron	Erythromycin	14B06-B35-290872	21669SI	43
Euro OTC	Erythromycin	1508034	21890SI	57

*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*.

- 126 484 spectra from a total of 2781 batches from further 781 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.

- 1831 spectra from 463 *Apo-Ident* customers from 429 batches from the substance/substance group *Erythromycin*.

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH, 4...	Erythromycin	10217208	1
Gehe	Erythromycin	11D13-N09	1
Caelo	Erythromycin	11j06-n05	1
Euro OTC	Erythromycin	700770	1
Euro OTC	Erythromycin	1106036-04	1
Caelo	Erythromycin	27071202	1
Caelo	Erythromycin	11195408	1
Fagron	Erythromycin	12E24-N04	14
Euro OTC	Erythromycin	1106036-05	6
Caelo	Erythromycin	11195407	3
Phagron	Erythromycin		1
Fagron	Erythromycin	EBS/1201-008	2
Fagron	Erythromycin	11D13-N09	2
Fagron	Erythromycin	11J06-N05	2
Fagron	Erythromycin	510211362	1
Noweda	Erythromycin	11195413	1
Caelo	Erythromycin	12152102	3
Caelo	Erythromycin	1195407	1
Eurompharm/Otto	Erythromycin	1106036-05	2
Caelo	Erythromycin	11195402	2
Noweda	Erythromycin	11195411	2
Caelo	Erythromycin	12152105	3
Fagron	Erythromycin	4212E-01362	1
VDL	Erythromycin	11195407	1
Anzag 23.11.12 ek:26,49	Erythromycin	1205035-01	1
Gehe	Erythromycin	12E24-N04	1
Caelo	Erythromycin	11195405	1
Fagron	Erythromycin	12J30-N01	12
Caelo	Erythromycin	12152109	10
Caelo	Erythromycin	1215219	1
Euro OTC	Erythromycin	1205035-01	13
Caelo	Erythromycin	20270912-3	1
Sanacorp	Erythromycin	1106036-04	1
Caelo	Erythromycin	12152202	3
Caelo	Erythromycin	12152205	10
Caelo	Erythromycin	3110195	1
EuRho	Erythromycin	1205035-01	1
Fagron	Erythromycin	13A02-N06	9
Noweda	Erythromycin	12152108	2
Caelo	Erythromycin	12152108	3
Caelo	Erythromycin	12E24-N04	1
Noweda	Erythromycin	12E24-N04	1
Caelo	Erythromycin	12152101	3
Anzag	Erythromycin	12152206	1
Euro OTC	Erythromycin	1205035-02	17

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Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	12152206	8
Euro OTC	Erythromycin	EBS/1205-M-040	1
Alliance Healthcare	Erythromycin	12E24-N04	1
Caelo	Erythromycin	13A02-N06	1
Euro OTC	Erythromycin	4112Q-01362	1
Fagron	Erythromycin	11J06-No5	1
Sanacorp	Erythromycin	12152202	1
Gehe	Erythromycin	12152105	1
Noweda	Erythromycin	12152201	1
Gehe	Erythromycin	12152108	1
Caelo	Erythromycin	22041302	1
Caelo	Erythromycin	12152201	7
Sanacorp	Erythromycin	1205035-02	1
Caelo	Erythromycin	12156201	3
Caelo	Erythromycin	12152208	4
Caelo	Erythromycin	12156202	7
Fagron	Erythromycin	E-250213-2	1
Fagron	Erythromycin	E-030613-1	1
Fagron	Erythromycin	13A02N06	1
Caelo	Erythromycin	12152104	2
Caelo	Erythromycin	12156208	6
Caelo	Erythromycin	12156207	3
Fagron	Erythromycin	13A02-No6	1
Fagron	Erythromycin	13A02-N060571/680	1
Phoenix	Erythromycin	12152201	2
Euro OTC	Erythromycin	1013u-01362	1
Fagron	Erythromycin	13d30-n01	1
Fagron	Erythromycin	13D30-N01	21
Caelo	Erythromycin	13D30-N01	3
Alliance Health	Erythromycin	120503502	1
Euro OTC	Erythromycin	1205036-01	7
Phönix	Erythromycin	121427016	1
Sanacorp	Erythromycin	12156208	1
Caelo	Erythromycin	19071306	1
Gehe	Erythromycin	1106036-05	1
Caelo	Erythromycin	12156206	2
Caelo	Erythromycin	1205036-01	2
Caelo	Erythromycin	11195306	1
Caelo	Erythromycin	13189001	7
Caelo	Erythromycin	12156204	4
Fagron	Erythromycin	13D30-N010336/730	1
Fagron	Erythromycin	13D30-N010278/730	1
Euro OTC	Erythromycin	12A02-N06	1
EuRho/Phönix	Erythromycin	1106036-05	1
Caelo	Erythromycin	1008018-02	1
Fagron	Erythromycin	13D30N01	1
EuRho	Erythromycin	1205035-02	1
Caelo	Erythromycin	13189002	7
Fagron	Erythromycin	12E24-No4	1
Euro OTC	Erythromycin	3613A1362	1
Caelo	Erythromycin	13175501	5
Caelo	Erythromycin	1315501	1
AHC 04.07.13 EK38,50	Erythromycin	12156207	1
Caelo	Erythromycin	13189004	5
Caelo	Erythromycin	13189007	1
Caelo	Erythromycin	13175502	4
Fagron	Erythromycin	1205036-01	1
Caelo	Erythromycin	13175603	10
Fagron	Erythromycin	13F12-N21	23
Caelo	Erythromycin	13175506	4

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Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	13189006	3
Noweda	Erythromycin	13175603	2
Euro OTC	Erythromycin	1205036-02	9
Caelo	Erythromycin	12152107	1
Caelo	Erythromycin	13175503	8
Caelo	Erythromycin	12156203	2
Caelo	Erythromycin	24101312	1
Caelo	Erythromycin	13175604	5
Caelo	Erythromycin	13175504-3413310132	1
Euro OTC	Erythromycin	120503602	2
Fagron	Erythromycin	13D30-N01003/456	1
Caelo	Erythromycin	511111	1
Fagron	Erythromycin	13A02-N-06	1
Caelo	Erythromycin	13175505	3
Caelo	Erythromycin	13175504	6
Fagron	Erythromycin	EB078B13	1
Euro CT Phönix	Erythromycin	13175604	1
Alliance Healthcare	Erythromycin	13F12-N21	1
Gehe	Erythromycin	13F12-N21	1
Euro OTC	Erythromycin	130801601	6
Caelo	Erythromycin	1308016-01	2
Euro OTC	Erythromycin	1308016-01	26
Fagron	Erythromycin	13175503	1
Caelo	Erythromycin	20122013D	1
Caelo	Erythromycin	13175601	10
EuRho/Phönix	Erythromycin	1205035	1
Euro OTC	Erythromycin	1205036/02	1
Caelo	Erythromycin	132152108	1
EuRho	Erythromycin	1205036-01	1
gepepharm GmbH	Erythromycin	13175502	1
Caelo	Erythromycin	59/AKD59	1
Caelo	Erythromycin	13175607	7
Phönix	Erythromycin	1205036-02	1
Fagron	Erythromycin	13H22-N07	4
fagr	Erythromycin	13A02-N06	1
Caelo	Erythromycin	13175612	2
Caeolo/Noweda	Erythromycin	13189007	1
Caelo	Erythromycin	13175804	2
Fagron	Erythromycin	13H22-N070126/246	1
Caelo	Erythromycin	13175506-3559412014	1
Sanacorp	Erythromycin	13H22-N07	1
Caelo	Erythromycin	13145504	1
Caelo	Erythromycin	131756017	1
Euro OTC	Erythromycin	120503502	1
Anzag	Erythromycin	13175506	1
Caesar&loretz,Phoenix	Erythromycin	13175602	1
Caelo	Erythromycin	13175802	7
Caelo	Erythromycin	13175801	9
Fagron	Erythromycin	13H22-N070228/246	1
Caelo	Erythromycin	13H22-N07	1
Caelo	Erythromycin	13175608	5
Fagron	Erythromycin	EB032J13	4
Noweda	Erythromycin	13175608	1
Fagron	Erythromycin	14B06-B35	10
Caelo	Erythromycin	13175803	6
Fagron	Erythromycin	14B06-B35-290875	5
Caelo	Erythromycin	13178756tzgklhj	1
Fagron	Erythromycin	14B06-B35-290873	2
Cealo / Noweda	Erythromycin	1205036-02	1
Caelo	Erythromycin	13175808	2

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Supplier	Substance	Batch	Spectra
Fagron	Erythromycin	13175608	1
Sanacorp	Erythromycin		1
Gutenberg-Apotheke	Erythromycin	13175608	1
Fagron	Erythromycin	14B06-B35-290874	3
Fagron	Erythromycin	14B06-B35290873	1
Caelo	Erythromycin	13175811	8
Fagron	Erythromycin	14B06-B35-290866	4
GEHE 21.05.2014	Erythromycin	1308016-01	1
Fagron	Erythromycin	13f12-n21	1
Fagron	Erythromycin	14b06-b35-290872	1
Caelo	Erythromycin	1114Q-01362	1
PHOENIX 08.05.2014	Erythromycin	13175608	2
PHOENIX 08.05.2014	Erythromycin	13175604	1
Caelo	Erythromycin	14044001	9
Euro OTC	Erythromycin	1308016-02	24
Fagron	Erythromycin	14B06-B35-290872	4
Fagron	Erythromycin	14B06-35-290873	1
Caelo	Erythromycin	13175809	5
Phoenix	Erythromycin	13175608	1
Phönix	Erythromycin	14B06-B35	1
Audor Pharma	Erythromycin	13175602	1
Caelo	Erythromycin	13175611	5
euroct/gehe	Erythromycin	1308016-01	1
euroct/gehe	Erythromycin	1308016-02	2
Caelo	Erythromycin	14044005	7
Caelo	Erythromycin	14044004	11
Euro	Erythromycin	1308016-02	1
Fagron	Erythromycin	14B06-B35-293509	6
Caelo	Erythromycin	3092014B	1
Euro OTC	Erythromycin	EBS/1307-BM-001	1
EuRho	Erythromycin	1308016-02	2
Fagron	Erythromycin	13175602	1
Caelo	Erythromycin	14044201	4
Caelo	Erythromycin	14044009	2
Sanacorp	Erythromycin	59/AKD51	1
Fagron	Erythromycin	14b06b5293508	1
Caelo	Erythromycin	14B06-B35-290872	1
Anzag	Erythromycin	14044001	1
Caelo	Erythromycin	1414M-01362	1
Caelo	Erythromycin	14b06-b35-293508	1
Caelo	Erythromycin	1308016-02	1
Bombastus	Erythromycin	14B06-B35-290873	1
Caelo	Erythromycin	14044002	7
Caelo	Erythromycin	14044007	7
Phönix	Erythromycin	14044201	1
Fagron	Erythromycin	14F13-B02-293488	3
Caelo	Erythromycin	14044010	4
Fagron	Erythromycin	13175803	1
Caelo	Erythromycin	1404409	1
EuRho/Phönix	Erythromycin	1308016-02	1
Euro OTC	Erythromycin	130801602	2
Caelo	Erythromycin	14044105	3
Fagron	Erythromycin	14F13-B02-293490	2
Fagron	Erythromycin	14F13-B02	2
Caelo	Erythromycin	14044008	4
Caesar&lorenz,Phoenix	Erythromycin	14044004	1
Gehe	Erythromycin	1308016-02	1
Noweda	Erythromycin	130801602	2
Caelo	Erythromycin	14044202	3
Caelo	Erythromycin	14044107	3

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Supplier	Substance	Batch	Spectra
Fagron	Erythromycin	14B06-B35-293508	2
Fagron	Erythromycin	13175810	1
	Erythromycin	1308016-02	1
Caelo	Erythromycin	14F13-B02-296464	2
Caelo	Erythromycin	14044006	6
Fagron	Erythromycin	14F13-B02-293487	1
Sanacorp;19.03.15;30,50EUR	Erythromycin	1409019-01	1
Caelo	Erythromycin	14044101	7
Fagron	Erythromycin	14I30-B01	5
Fagron	Erythromycin	14F13-B02-293511	2
Caelo	Erythromycin	14044115	6
Caelo	Erythromycin	14I30-B01	1
Euro OTC	Erythromycin	1409019-01	22
OTG/Gehe	Erythromycin	1409019-01	1
Gehe	Erythromycin	1409019-01	3
Fagron	Erythromycin	14F13-B02-296464	2
Caelo	Erythromycin	14044109	5
Caelo	Erythromycin	13175810	2
Fagron	Erythromycin	EB022E14	2
Fagron	Erythromycin	14I30-B01-300062	2
Caelo	Erythromycin	140440044	1
Noweda	Erythromycin	14044006	1
Eigenherstellung	Erythromycin	14044006	1
Caelo	Erythromycin	5052015D	1
Noweda21.04.2015	Erythromycin	14044110	1
Euro OTC	Erythromycin	140901901	3
Euro OTC	Erythromycin	1409019-01Mg100g	1
Caelo	Erythromycin	14F13-B02-300061	1
Caelo	Erythromycin	1430b01300059	1
Euro OTC	Erythromycin	14044205	1
Fagron	Erythromycin	14/30-B01-300060	3
Caelo	Erythromycin	14044205	4
Fagron	Erythromycin	14I30-B01-300060	2
Caelo	Erythromycin	14044106	1
Caelo	Erythromycin	14044114	5
Fagron	Erythromycin	14i30b01-300059	1
Caelo	Erythromycin	14044110	1
Caelo	Erythromycin	14044118	3
Caelo	Erythromycin	14044012	2
Fagron	Erythromycin	14/30B01300060	1
Fagron	Erythromycin	14I30B01	1
Fagron	Erythromycin	14F13-B12-300061	1
Caelo	Erythromycin	14044206	2
Fagron	Erythromycin	14I30-B01-300063	1
Caelo	Erythromycin	14/30-B01-300059	1
Fagron	Erythromycin	14I30-B01-300060	1
Caelo	Erythromycin	1409019-01	2
Caelo	Erythromycin	15042601	2
Caelo	Erythromycin	14044014	2
Fagron	Erythromycin	14F13-B02-300061	2
Caelo	Erythromycin	14044207	1
Fagron	Erythromycin	14/30B01300050	1
Fagron	Erythromycin	14I30-B01-303884	5
Caelo	Erythromycin	1404418	1
Euro OTC	Erythromycin	1409019-02	42
Calo/AHD	Erythromycin	15042605	1
Caelo	Erythromycin	15042605	5
Caelo	Erythromycin	14044011	2
Caelo	Erythromycin	15042602	5
Fagron	Erythromycin	1430B01303884	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Erythromycin	140919-02	1
Euro OTC	Erythromycin	140901902	1
Fagron	Erythromycin	14/30-B01	1
Fagron	Erythromycin	14I30-B01-300050	1
caesar&loretz,phönix	Erythromycin	15042603	1
Caelo	Erythromycin	15042612	6
Caelo	Erythromycin		3
Caelo	Erythromycin	14/30-B01-308189	2
Caelo	Erythromycin	15042702	4
EurPS	Erythromycin	1409019-02	3
Caelo	Erythromycin	15042610	10
Euro OTC	Erythromycin	14090-9-01	1
Caelo	Erythromycin	15042604	3
Fagron	Erythromycin	1409019-02	2
Fagron	Erythromycin	EB068/14	1
Fagron	Erythromycin	3000-50	1
Caelo	Erythromycin	EB06/14	1
Fagron	Erythromycin	14/30-B01-308789	3
Fagron	Erythromycin	EB06814	1
Caelo	Erythromycin	15042603	4
Caelo	Erythromycin	15042701	7
EuroTOC / Noweda	Erythromycin	1409019-02	1
Caelo	Erythromycin	15042613	3
Noweda	Erythromycin	14044114	1
Euroct/Gehe	Erythromycin	1409019-01	2
Bombastus	Erythromycin	15042603	1
Caelo	Erythromycin	15042703	7
Fagron	Erythromycin	14I30-B01-306927	3
Caelo	Erythromycin	1404414	1
Caelo	Erythromycin	15042707	1
Caelo	Erythromycin	15042706	7
Caelo	Erythromycin	15042705	11
Gehe	Erythromycin	15042603	1
Caelo	Erythromycin	15042609	8
Fagron	Erythromycin	14I30-B01-308189	1
Caelo	Erythromycin	15042704	6
Euro OTC	Erythromycin	1508034-01	31
Fagron	Erythromycin	1430-B01-308789	1
Fagron	Erythromycin	14/30-B01308790	1
Bombastus	Erythromycin	14F13-B02	1
Fagron	Erythromycin	14I30-B01-308188	4
Caesar&Loretz GmbH / Anzag	Erythromycin	15042610	1
Fagron	Erythromycin	1430-b01-300060	1
Fagron	Erythromycin	14I30-B01-311166	2
Fagron	Erythromycin	14I30-B01-308789	1
Gehe	Erythromycin	15042705	1
Caelo	Erythromycin	15042606	1
Euro/Gehe	Erythromycin	1508034-01	1
Caelo	Erythromycin	15245101	7
Fagron	Erythromycin		2
Euro OT	Erythromycin	1409019-02	1
Caelo	Erythromycin	15042611	5
Fagron	Erythromycin	14/30-B01-308189	2
Noweda	Erythromycin	15245101	1
Fagron	Erythromycin	15G07-B05-312356	2
Caelo	Erythromycin	140901902	2
Euro OTC	Erythromycin	150803401	1
Fagron	Erythromycin	14i30-b01-311166	1
Hedinger	Erythromycin	15245002	2
Fagron	Erythromycin	14I30B01308189	1

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Supplier	Substance	Batch	Spectra
Noweda/Gehe	Erythromycin	14B06-B35-293508	1
Caelo	Erythromycin	15245004	9
phönix	Erythromycin	15245101	1
Caelo	Erythromycin	15042611-20160504Ma1	1
Euro OTC	Erythromycin	15080-01	1
Fagron	Erythromycin	1508034-01	2
Caelo	Erythromycin	1524002	1
phönix	Erythromycin	15042611	1
Wolff/AHD	Erythromycin	15245004	1
Caelo	Erythromycin	15042711	9
Caelo	Erythromycin	15245003	7
Caelo	Erythromycin	15245002	15
Klenk	Erythromycin	EB068I14	1
Phoenix	Erythromycin	15042609	1
Euro OTC	Erythromycin	1508034-02	12
Euro OTC	Erythromycin	80616-4	1
Caelo	Erythromycin	150803401	1
Caelo	Erythromycin	15042803	10
EuRho/Noweda	Erythromycin	1508034-02	1
Caelo	Erythromycin	1508034-02	3
Unisan	Erythromycin	140901902	1
Fagron	Erythromycin	1430-B01-303884	1
Euro OTC	Erythromycin	1508034-02Mg100g	1
Noweda	Erythromycin	150803401	1
Caelo	Erythromycin	15042802	3
Biomed	Erythromycin	1508035-01	1
Caelo	Erythromycin	1409019-02	1
Caelo	Erythromycin	3081601	1
Phönix WE:30.07.2016 ...	Erythromycin	15245101	1
Euro OTC	Erythromycin	15042810	1
Caelo	Erythromycin	15042808	1
Caelo	Erythromycin	15245008	3
Caelo	Erythromycin	15245007	2
Caelo	Erythromycin	15042608	3
Phoenix	Erythromycin	15042811	1
Caelo	Erythromycin	15042809	3
Fagron	Erythromycin	14/30-B01-303884	1
Caelo	Erythromycin	15245005	1
Caelo	Erythromycin	1524004	1
Caelo	Erythromycin	15042810	2
Caelo	Erythromycin	15042811	3
Fagron	Erythromycin	16G06-B03-324466	5
Fagron	Erythromycin	16G06-B03-324463	6
Caelo	Erythromycin	15042806	10
Caesar&Loretz GmbH	Erythromycin	15042807	1
Fagron	Erythromycin	16G06-B03-324464	11
Caelo	Erythromycin	150428	1
Caelo	Erythromycin	15042813	10
Fagron	Erythromycin	16G06-B03-324463	1
Euro OTC	Erythromycin	1607038-01	48
Caelo	Erythromycin	16079202	5
Caelo	Erythromycin	140930E	1
Caelo	Erythromycin	16079201	5
Caelo	Erythromycin	15042902	2
Caelo	Erythromycin	160703801	1
Ichthyol-Gesellschaft	Erythromycin	161020E/1607038-01	1
Fagron	Erythromycin	0EBA/0010516	2
Fagron	Erythromycin	16G06-B03-324465	4
Fagron	Erythromycin	16G06-B03	5
Fagron	Erythromycin	16g06-b03-324463	2

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Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	16G06-B03-324465	1
Gehe	Erythromycin	15245004	1
phönix	Erythromycin	15042813	1
Caelo	Erythromycin	1504813	1
Caelo	Erythromycin	1607038-01	1
Caelo	Erythromycin	15042901	6
Caesar & Loretz/AHC	Erythromycin	15042813	1
Caelo	Erythromycin	16079208	5
Caelo	Erythromycin	16079203	16
Caelo	Erythromycin	1181116	1
Caelo	Erythromycin	1171116	1
Caelo	Erythromycin	15042816	3
Euro OTC	Erythromycin	160703801	4
Jenapharm/Phönix	Erythromycin	1607036-01	1
Caelo	Erythromycin	16979201	1
Alte Apotheke	Erythromycin	16079206	1
Caelo	Erythromycin	15042814	8
Caelo	Erythromycin	16079204	9
AHD 26.02.16 13,15EUR	Erythromycin	14I30-B01-308789	1
Caelo	Erythromycin	15042812	1
Caelo	Erythromycin	16079213	9
Euro OTC	Erythromycin	1607038	1
GEHE	Erythromycin	16079208	1
Euro OTC	Erythromycin	167038-01	1
Fagron	Erythromycin	16079208	1
Noweda/Euro	Erythromycin	1607038-01	2
Caelo	Erythromycin	16079210	8
Caelo	Erythromycin	16G06-803	1
Fagron	Erythromycin	16G06-B030003	1
Euro OTC	Erythromycin	1607038-02	36
Fagron	Erythromycin	16G06-B03-324462	2
AIH	Erythromycin	15042902	1
Caelo	Erythromycin	16079501	10
Phönix	Erythromycin	16079205	1
Caelo	Erythromycin	16079205	2
Gehe	Erythromycin	16079209	1
Caesar & Loretz GmbH	Erythromycin	15042814	1
VDL	Erythromycin	160703801	1
Caelo	Erythromycin	16079214	8
Caelo	Erythromycin	16079505	2
Caelo	Erythromycin	1607038-02	5
Caelo	Erythromycin	16079216	6
Caelo	Erythromycin	15042815	3
Caelo	Erythromycin	16079207	4
Caelo	Erythromycin	16079511	4
Gehe	Erythromycin	16079204	1
Caelo	Erythromycin	16079602	4
Euro OTC	Erythromycin	1607038-2	1
Krieger	Erythromycin	16G06-B03-329150	1
Fagron	Erythromycin	16G06-B03-329149	3
Caelo	Erythromycin	16079506	3
Fagron	Erythromycin	16G06-B03-329150	3
GEHE	Erythromycin	16079213	2
Caelo	Erythromycin	16079513	8
Allianz Healthcare	Erythromycin	16079602	1
Fagron	Erythromycin	16G06-B03324464	1
Euro OTC	Erythromycin	16079206	1
Anzag	Erythromycin	16079501	1
Finteler Apotheke	Erythromycin	1607038-02	1
Caelo	Erythromycin	16079502	7

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Supplier	Substance	Batch	Spectra
Biomed/Phönix	Erythromycin	1607038-01	1
Euro OTC	Erythromycin	1607038/01	1
Caelo	Erythromycin	16079515	1
Caelo	Erythromycin	16G06B03329150	1
Fagron	Erythromycin	16/24-B10-329158	1
Gehe	Erythromycin	16G06-B03	1
Phoenix	Erythromycin	16079501	1
Caelo	Erythromycin	16079214-20170704Ma1	1
Fagron	Erythromycin	16J24-B10-329154	1
Caelo	Erythromycin	16079503	3
Fagron	Erythromycin	16g06-b03-329150	1
Gehe	Erythromycin	1607038-02	1
Caelo	Erythromycin	16079512	2
Caelo	Erythromycin	16079510	2
Fagron	Erythromycin	16G06B03-329149	1
Caelo	Erythromycin	16079603	6
Euro OTC	Erythromycin	160703802	2
Caelo	Erythromycin	16079608	9
Noweda	Erythromycin	1607038-02	1
Caelo	Erythromycin	160796	1
Fagron	Erythromycin	16G06-B03-329157	2
GEHE	Erythromycin	16079512	1
Fagron	Erythromycin	16J24-B10-329156	6
Euro OTC	Erythromycin	1705038-01	46
Noweda	Erythromycin	16079606	1
Caelo	Erythromycin	16079612	10
Fagron	Erythromycin	16J25-B10-329155	1
Caelo	Erythromycin	16079604	2
Caelo	Erythromycin	16079606	3
Fagron	Erythromycin	16J24-B10-329155	2
Caelo	Erythromycin	16079509	3
Caelo	Erythromycin	16079514	1
Bombastus	Erythromycin	16079606	1
Fagron	Erythromycin	16079608	1
Phönix WE: 23.09.17 E...	Erythromycin	16079604	1
gehe	Erythromycin	1607038-02	2
Caesar & Loretz GmbH, P...	Erythromycin	16079207	1
Caelo	Erythromycin	16079605	2
Caelo	Erythromycin	16079607	1
Caelo	Erythromycin	1708807	1
Caelo	Erythromycin	16079609	2
Fagron	Erythromycin	16J24-B10-329158	2
Caelo	Erythromycin	16079206	1
Fargon/Sanacorp	Erythromycin	16J24-B10-329158	1
Fagron	Erythromycin	16J24-B10-3367363	1
GEHE	Erythromycin	16079609	2
Caelo	Erythromycin	16079702	6
Fagron	Erythromycin	16j24-b10-329155	1
Caelo	Erythromycin	16079214-20171127Ma6	1
Caelo	Erythromycin	17088007	7
Gehe	Erythromycin	16079510	1
Fagron	Erythromycin	0EBA/0020516	2
Caelo	Erythromycin	17088002	11
Fagron	Erythromycin	16J24-B10-339487	5
Caeolo/Krieger	Erythromycin	17088004	1
Caelo	Erythromycin	16079610	1
Caelo	Erythromycin	17088003	3
Caelo	Erythromycin	17088004	2
Caelo	Erythromycin	16G06-B03-324466	1
Sanacorp	Erythromycin	16J24-B10	2

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Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	17088010	6
Euro OTC	Erythromycin	EBS/1701-BM-001	3
Fagron	Erythromycin	16J24-B10	1
Caelo	Erythromycin	17088008-E20180112Ma	1
Caelo	Erythromycin	17088008	5
Gehe	Erythromycin	16J24-B10-336735	1
Sanacorp	Erythromycin	17088002	1
Noweda	Erythromycin	17088003	1
Caelo	Erythromycin	17088402	3
Fagron	Erythromycin	16J24-B10-336735	4
Euro OTC	Erythromycin	180201E/1705038-01	1
Caelo	Erythromycin	17088009	4
Caelo	Erythromycin	17088008-20180206Ma2	1
Fagron	Erythromycin	16/24-B10-339487	2
Caelo	Erythromycin	1705038-01	2
Caelo	Erythromycin	17088013	4
Noweda	Erythromycin	16J24-B10	1
Krieger	Erythromycin	16J24-B10-336735	1
Phoenix/Cealo	Erythromycin	17088004/0918E-01362	1
Fagron	Erythromycin	17088402	1
Caelo	Erythromycin	17088001	2
Caelo	Erythromycin	17088301	18
EuRho/Noweda	Erythromycin	1705038-01	1
Caelo	Erythromycin	17088401	1
Euro OTC	Erythromycin	1508034	1
Caelo	Erythromycin	17088010-20180404Ma2	1
Caelo	Erythromycin	17088403	5
Caelo	Erythromycin	17088405	3
Fagron	Erythromycin	16J24-B10-341875	2
Sanacorp	Erythromycin	17088203	2
Caelo	Erythromycin	17088204	10
Caelo	Erythromycin	178824	1
GEHE	Erythromycin	17088008	1
Euro OTC	Erythromycin	17088203	2
Caelo	Erythromycin	17088403-20180619Ma1	1
Caelo	Erythromycin	16J24-B10-341875	1
Fagron	Erythromycin	16J24-B10-339488	2
Fagron	Erythromycin	1705038-01	1
Fagron	Erythromycin	700770-0002	1
Caelo	Erythromycin	17088203	4
Fagron	Erythromycin	16J24-B10-346206	2
Kehr	Erythromycin	1705038-01	1
Caelo	Erythromycin	170718A	1
Krieger	Erythromycin	16J24-B10-341876	1
Euro OTC	Erythromycin	1705038-02	4
Fagron	Erythromycin	16/24-B10-341875	1
Caelo	Erythromycin	17088406	3
Caelo	Erythromycin	170880103	1
Caelo	Erythromycin	16J24-B-341876	1
Fagron	Erythromycin	18F05-B01-350906	1
Caelo	Erythromycin	17088210	3
Fagron	Erythromycin	CEPEB001E18	1
Fagron	Erythromycin	18F-05-B01	1
Caelo	Erythromycin	17088210-E20181115Ma	1
Caelo	Erythromycin	17088403-E2081115Ma1	1
Euro OTC	Erythromycin	1705038-03	5
Gehe	Erythromycin	18F05-B01-352501	1
Fagron	Erythromycin	17088211	1
Euro OTC	Erythromycin	170503803	1
Caelo	Erythromycin	17088302	1

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Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	17088306	2
Euro OTC	Erythromycin	17088005	1
Caelo	Erythromycin	17088305	1
Sanacorp	Erythromycin	17088302	1
Caelo	Erythromycin	17088005	1
Caelo	Erythromycin	1708/8308	1
Fagron	Erythromycin	18f05-b01-350908	1
Fagron	Erythromycin	18f05-b01-352501	1
Caelo	Erythromycin	18096201	1
Caelo	Erythromycin	17088309	1
Fagron	Erythromycin	18F05-B01-352500	1

- 77 098 spectra from 565 *Apo-Ident* customers from a total of 25 712 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	380	0	74 116
Type B	0	401	7	126 484
Type C	0	1826	5	77 098

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9901 %)	98.2843 % (> 97.5490 %)
Type C	100.0000 % (> 99.8817 %)	99.7269 % (> 99.5631 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21323	21890	3.16	33.96
21056	21890	7.92	36.67
21651	21651	0.00	33.24
23438	23438	0.00	40.23
24420	24420	0.00	32.86
21669	24420	10.04	34.73
21890	21890	0.00	33.10
22832	22832	0.00	40.71
22438	22438	0.00	33.11

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Estradiol benzoate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20098-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Estradiol benzoate; Estradioli benzoas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Estradiol benzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Estradiol benzoate	12H02-N02	20889	40	20120817
Fagron	Estradiol benzoate	14B20-B02	21257	40	20140327
Euro OTC	Estradiol benzoate	1301006-02	21290	40	1507405
Euro OTC	Estradiol benzoate	1507009	21869	40	0000010566
Caello	Estradiol benzoate	15078608	23218	40	20150415

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Estradiol benzoate	12H02-N02	20889SI	40	20120817
Fagron	Estradiol benzoate	14B20-B02	21257SI	40	20140327
Euro OTC	Estradiol benzoate	1507009	21869SI	40	0000010566

Validation samples

A total of 280317 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 *Estradiol benzoate*. These samples are listed above in the [calibration samples](#) section.
- 74176 spectra from a total of 1618 batches from further 372 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 [†].

- 400 spectra of 12 reference samples from the substance/substance group *Estradiol benzoate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estradiol benzoate	13277607	21324	40
Euro OTC	Estradiol benzoate	1507009	21869 [†]	20
Euro OTC	Estradiol benzoate	1611004	22873	40
Euro OTC	Estradiol benzoate	1412033	24139	40
Caelo	Estradiol benzoate	181444	24254	40
Fagron	Estradiol benzoate	12H02-N02	20889SI [†]	20
Fagron	Estradiol benzoate	14B20-B02	21257SI [†]	20
Euro OTC	Estradiol benzoate	1507009	21869SI [†]	20
Euro OTC	Estradiol benzoate	1611004	22873SI	40
Caelo	Estradiol benzoate	15078608	23218SI	40
Euro OTC	Estradiol benzoate	1412033	24139SI	40
Caelo	Estradiol benzoate	181444	24254SI	40

- 126492 spectra from a total of 2781 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the

[†]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.

- 290 spectra from 190 *Apo-Ident* customers from 79 batches from the substance/substance group *Estradiol benzoate*.

Supplier	Substance	Batch	Spectra
Caelo	Estradiol benzoate	10124915	2
Euro OTC	Estradiol benzoate	1007037-02	1
Gehe	Estradiol benzoate	11L23-N01	1
Finze	Estradiol benzoate	1003040-01	2
Euro OTC	Estradiol benzoate	1201019-01	7
Fagron	Estradiol benzoate	11L23-N01	1
Caelo	Estradiol benzoate	10124918	2
Caelo	Estradiol benzoate	10124921	1
Caelo	Estradiol benzoate	12255904	10
Caelo	Estradiol benzoate	10124909	5
Euro OTC	Estradiol benzoate	1201019-02	9
Euro OTC	Estradiol benzoate	121019-01	1
Caelo	Estradiol benzoate		4
Caelo	Estradiol benzoate	10124919	1
Caelo	Estradiol benzoate	12255905	10
Caelo	Estradiol benzoate	10124912	1
Fagron	Estradiol benzoate	12H02-N02	3
A.H. 07.06.13 ek: 24,14EUR	Estradiol benzoate	1201019-02	1
Caelo	Estradiol benzoate	92137389	1
Fagron	Estradiol benzoate	12H02-N052	1
Euro OTC	Estradiol benzoate	1301006-01	2
Euro OTC	Estradiol benzoate	130100601	1
Caelo	Estradiol benzoate	6091305	1
Fagron	Estradiol benzoate	2x12L14-N02	1
Fagron	Estradiol benzoate	12L14-N02	1
Caelo	Estradiol benzoate	13277602	8
Fagron	Estradiol benzoate	13I11-N01	1
Alliance Healthcare	Estradiol benzoate	1301006-01	1
Caelo	Estradiol benzoate	81403700	1
Sanacorp	Estradiol benzoate	10/AKD24	1
Fagron	Estradiol benzoate	13I11N01	1
Bayer-Schering	Estradiol benzoate	1007037-03	1
Fagron	Estradiol benzoate	81403680	1
Fagron	Estradiol benzoate	13/11-N01	2
Caelo	Estradiol benzoate	13276401	6
alliance healthcare 5.12...	Estradiol benzoate	10118576	1
Noweda	Estradiol benzoate	13277603	1
Caelo	Estradiol benzoate	13277603	2
Euro OTC	Estradiol benzoate	8011422	1
Euro OTC	Estradiol benzoate	1301006-02	9
Caelo	Estradiol benzoate	21121204	1
Fagron	Estradiol benzoate	81403690	2
EuRho/Sanacorp	Estradiol benzoate	1201019-02	1
Caelo	Estradiol benzoate	13277605	3
Fagron	Estradiol benzoate	13C15-B07-288645	1
Caelo	Estradiol benzoate	13277607	3
Caelo	Estradiol benzoate	1301006-02	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Estradiol benzoate	1401001-01	9
Fagron	Estradiol benzoate	14B20-B02-292001	5
Euro OTC	Estradiol benzoate	14010001-01	1
Euro OTC	Estradiol benzoate	140101-01	1
AHD	Estradiol benzoate	14B20-B02-292001	1
VDI 16.10.14 12,70 euro	Estradiol benzoate		1
Fagron	Estradiol benzoate	14B20-B02-2920001	1
Caelo	Estradiol benzoate	1149	1
Fagron	Estradiol benzoate	14B20-B02-294949	2
Euro OTC	Estradiol benzoate	83101340	1
Fagron	Estradiol benzoate	83101340	2
Fagron	Estradiol benzoate	14B20-B02	3
Fagron	Estradiol benzoate	14b20-b02-294949	1
Bayer Pharma/Noweda	Estradiol benzoate	14B20-B02-292001	1
phönix	Estradiol benzoate	14B20-B02-294949	1
Euro OTC	Estradiol benzoate	1412033-01	8
Fagron	Estradiol benzoate	1412033-01	1
Fagron	Estradiol benzoate	15C10-B04-305523	6
Caelo	Estradiol benzoate	15078602	6
Euro OTC	Estradiol benzoate	84303830	1
Caelo	Estradiol benzoate	15078604	17
Caelo	Estradiol benzoate	15C10-B04-305523	2
Euro OTC	Estradiol benzoate	1507009-01	13
Caelo	Estradiol benzoate	84303830	1
Caelo	Estradiol benzoate	15078603	15
Caelo	Estradiol benzoate	15C10B04305523	1
sanacorp	Estradiol benzoate	15078604	1
Fagron	Estradiol benzoate	84303830	1
Euro OTC	Estradiol benzoate	150700901	2
Fagron	Estradiol benzoate	12D20N06	1
Fagron	Estradiol benzoate	12B08-N05	1
Caelo	Estradiol benzoate	1201019-02	1
Fagron	Estradiol benzoate	15c10-b04-305523	1
WE:Phönix 21.09.2012	Estradiol benzoate	12B08-N05	1
Fagron	Estradiol benzoate	15E08-B08-311705	8
Caelo	Estradiol benzoate	150918EB	1
Caelo	Estradiol benzoate	15078606	4
Caelo	Estradiol benzoate	1507806	1
Caelo	Estradiol benzoate	15078608	11
VDL	Estradiol benzoate	1507009-01	1
Caelo	Estradiol benzoate	1507009-01	1
Caelo	Estradiol benzoate	1401001-01	1
Gehe	Estradiol benzoate	15078606	1
Caelo	Estradiol benzoate	1100417	1
Caelo	Estradiol benzoate	16003701	4
Noweda	Estradiol benzoate	15078608	1
Euro OTC	Estradiol benzoate	1611004-01	5
Phönix	Estradiol benzoate	16003707	1
Phoenix WE:20.11.17 1g/...	Estradiol benzoate	16003702	1
Caelo	Estradiol benzoate	16003707	7
Caelo	Estradiol benzoate	16003702	1
Phoenix/Cealo	Estradiol benzoate	1611004-01	1
Bayer Pharma AG / Noweda	Estradiol benzoate	14B20-B02	1
Caelo	Estradiol benzoate	18144402	5
Euro OTC	Estradiol benzoate	161100402	1
Fagron	Estradiol benzoate	17357602	1
Euro OTC	Estradiol benzoate	1807161	1

- 78 639 spectra from 565 *Apo-Ident* customers from a total of 26 059 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Estradiol 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 *Estradiol 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	320	0	74 176
Type B	0	400	0	126 492
Type C	0	231	59	78 639

The substance/substance group *Estradiol 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 % (> 99.9887 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.5000 %)
Type C	100.0000 % (> 99.8817 %)	79.6552 % (> 78.6207 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21257	21290	1.85	65.43
21290	21290	0.00	61.70
20889	21290	2.75	65.34
21869	21869	0.00	55.46
23218	21869	5.75	64.65

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Estradiol hemihydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20497-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Estradiol hemihydrate; Estradiolum hemihydricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Estradiol hemihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Estradiol hemihy...	1208022-01	21291	40	20121012
Caelo	Estradiol hemihy...	12268016	21302	40	1410502
Caelo	Estradiol hemihy...	13285802	21508	40	1410504
Fagron	Estradiol hemihy...	14G24-B04-297404	21667	40	20140825
Euro OTC	Estradiol hemihy...	1507013	21847	40	1510623

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Estradiol hemihy...	1510039	21945	40	20151103*
Euro OTC	Estradiol hemihy...	1601017	22307	30	20160122*
Euro OTC	Estradiol hemihy...	1612008	22913	40	20170117*
Fagron	Estradiol hemihy...	16H04-B01-328738	23184	40	20160915
Euro OTC	Estradiol hemihy...	1507013	21847SI	40	1510623
Euro OTC	Estradiol hemihy...	1510039	21945SI	69	20151103*
Euro OTC	Estradiol hemihy...	1612008	22913SI	40	20170117*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 499 spectra of 12 reference samples from the substance/substance group *Estradiol hemihydrate*. These samples are listed above in the [calibration samples](#) section.
- 73997 spectra from a total of 1614 batches from further 372 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 [†].

- 1535 spectra of 48 reference samples from the substance/substance group *Estradiol hemihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Estradiol hemihydrate	13K22-N01	21263	40
Caelo	Estradiol hemihydrate	13285802	21499	60
Caelo	Estradiol hemihydrate	13285802	21500	60
Caelo	Estradiol hemihydrate	13285802	21501	20
Caelo	Estradiol hemihydrate	13285802	21502	20
Caelo	Estradiol hemihydrate	13285802	21503	20
Caelo	Estradiol hemihydrate	13285802	21504	20
Caelo	Estradiol hemihydrate	13285802	21505	20
Caelo	Estradiol hemihydrate	13285802	21506	20
Caelo	Estradiol hemihydrate	13285802	21507	20
Caelo	Estradiol hemihydrate	13285802	21508 [†]	20
Fagron	Estradiol hemihydrate	14G24-B04-297404	21667 [†]	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
Euro OTC	Estradiol hemihydrate	1507013	21847 [†]	20
Euro OTC	Estradiol hemihydrate	1510039	21945 [†]	20
Euro OTC	Estradiol hemihydrate	1601017	22307 [†]	15
Euro OTC	Estradiol hemihydrate	1607003	22712	40
Euro OTC	Estradiol hemihydrate	1612008-01	23099	40
Caelo	Estradiol hemihydrate	170582	23339	40
Euro OTC	Estradiol hemihydrate	1705018	23431	40
Euro OTC	Estradiol hemihydrate	1710031	23779	40
Euro OTC	Estradiol hemihydrate	1802013	24083	40
Euro OTC	Estradiol hemihydrate	1802012	24086	40
Caelo	Estradiol hemihydrate	181443	24257	40
Euro OTC	Estradiol hemihydrate	1809022	24319	40
Euro OTC	Estradiol hemihydrate	1808032	24322	40
Caelo	Estradiol hemihydrate	13285802	21499SI	60
Caelo	Estradiol hemihydrate	13285802	21500SI	60
Caelo	Estradiol hemihydrate	13285802	21501SI	20
Caelo	Estradiol hemihydrate	13285802	21502SI	20
Caelo	Estradiol hemihydrate	13285802	21503SI	20
Caelo	Estradiol hemihydrate	13285802	21504SI	20
Caelo	Estradiol hemihydrate	13285802	21505SI	20
Caelo	Estradiol hemihydrate	13285802	21506SI	20
Caelo	Estradiol hemihydrate	13285802	21507SI	20
Euro OTC	Estradiol hemihydrate	1507013	21847SI [†]	20
Euro OTC	Estradiol hemihydrate	1510039	21945SI [†]	20
Euro OTC	Estradiol hemihydrate	1601017	22307SI	45
Euro OTC	Estradiol hemihydrate	1607003	22712SI	40
Euro OTC	Estradiol hemihydrate	1612008-01	23099SI	30
Fagron	Estradiol hemihydrate	16H04-B01-328738	23184SI	30
Caelo	Estradiol hemihydrate	170582	23339SI	30
Euro OTC	Estradiol hemihydrate	1705018	23431SI	30
Euro OTC	Estradiol hemihydrate	1710031	23779SI	40
Euro OTC	Estradiol hemihydrate	1802013	24083SI	40
Euro OTC	Estradiol hemihydrate	1802012	24086SI	40
Caelo	Estradiol hemihydrate	181443	24257SI	40
Euro OTC	Estradiol hemihydrate	1809022	24319SI	40
Euro OTC	Estradiol hemihydrate	1808032	24322SI	40

- 125 357 spectra from a total of 2772 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 134 spectra from 83 *Apo-Ident* customers from 70 batches from the substance/substance group *Estradiol hemihydrate*.

[†]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
Fagron	Estradiol hemihydrate	12F29-N03	6
Fagron	Estradiol hemihydrate	9J27-N05	1
Caelo	Estradiol hemihydrate	11078113	1
Caelo	Estradiol hemihydrate	11078104	1
Caelo	Estradiol hemihydrate	12F29-N03	1
Fagron	Estradiol hemihydrate	12L19-N07	6
Fagron	Estradiol hemihydrate	11H23-N02	1
Caelo	Estradiol hemihydrate	12268003	1
Fagron	Estradiol hemihydrate	9G07N01	1
Caelo	Estradiol hemihydrate	12172003	2
Fagron	Estradiol hemihydrate	13E07-N02	3
Noweda	Estradiol hemihydrate	12268008	1
Gehe	Estradiol hemihydrate	82404160	1
Fagron	Estradiol hemihydrate	12L29-N07	1
Caelo	Estradiol hemihydrate	22101301	1
Caelo	Estradiol hemihydrate	9248916	2
Caelo	Estradiol hemihydrate	12268012	4
Fagron	Estradiol hemihydrate	13K22-N01	5
Euro OTC	Estradiol hemihydrate	1308003-01	2
Caelo	Estradiol hemihydrate	13285801	1
Fagron	Estradiol hemihydrate	11031401	1
Bayer Pharma	Estradiol hemihydrate	13K22-N01	2
Fagron	Estradiol hemihydrate	13K22N01	1
Caelo	Estradiol hemihydrate	11078105	1
Caelo	Estradiol hemihydrate	13285802	4
Fagron	Estradiol hemihydrate	83100820	2
Euro OTC	Estradiol hemihydrate	1404030-01	1
Fagron	Estradiol hemihydrate	13k22n01	1
Fagron	Estradiol hemihydrate	14G24-B04-297402	2
phönix	Estradiol hemihydrate	13285802	1
Fagron	Estradiol hemihydrate	14G24-B04-297406	1
Fagron	Estradiol hemihydrate	14G24-B04-297405	1
Caelo	Estradiol hemihydrate	13285811	3
Fagron	Estradiol hemihydrate	11A21-N01	1
Caelo	Estradiol hemihydrate	19051501	1
Fagron	Estradiol hemihydrate	14G24-B04-297404	1
Fagron	Estradiol hemihydrate	84201170	1
Noweda	Estradiol hemihydrate	15038004	1
Fagron	Estradiol hemihydrate	14G24-B04-302446	3
Fagron	Estradiol hemihydrate	15D01-B02-308190	1
Anzag; 12.72EUR; 7.10.2015	Estradiol hemihydrate	15038004	1
Bayer Pharma AG	Estradiol hemihydrate	1411024-01	2
Fagron	Estradiol hemihydrate	302446	1
Caelo	Estradiol hemihydrate	15038004	5
Euro OTC	Estradiol hemihydrate	1411024-01	2
Caelo	Estradiol hemihydrate	15038010	2
Euro OTC	Estradiol hemihydrate	1504034-01	1
Fagron	Estradiol hemihydrate	15D01-B02-308568	1
Euro OTC	Estradiol hemihydrate	1601017-01	1
Caelo	Estradiol hemihydrate	1601017-01	5
Caelo	Estradiol hemihydrate	1503801	1
Caelo	Estradiol hemihydrate	84201560	1
Fagron	Estradiol hemihydrate	15D01-B02-312068	2
Sanacorp	Estradiol hemihydrate	15038010	1
Fagron	Estradiol hemihydrate	15D01-B02-319032	1
Caelo	Estradiol hemihydrate	15D01-B02-319032	1
Caelo	Estradiol hemihydrate	15038014	2
Fagron	Estradiol hemihydrate	84201560	1
Euro OTC	Estradiol hemihydrate	1607003-01	2
Gehe	Estradiol hemihydrate	15038016	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Estradiol hemihydrate	1607003-0101374814	1
Caelo	Estradiol hemihydrate	15D01-B02-322166	1
Fagron	Estradiol hemihydrate	16h04-b01-328738	1
Caelo	Estradiol hemihydrate	15385410	1
Fagron	Estradiol hemihydrate	16H04-B01-328738	1
Euro OTC	Estradiol hemihydrate	15D01-B02	1
Fagron	Estradiol hemihydrate	16D12-B01-326783	4
Euro/ Phönix	Estradiol hemihydrate	3417M-02845	1
Euro OTC	Estradiol hemihydrate	17058205	1
Fagron	Estradiol hemihydrate	16h04-b01-334200	1
Euro OTC	Estradiol hemihydrate	1612008-01	1
Fagron	Estradiol hemihydrate	16H04-B01-339490	1
Caelo	Estradiol hemihydrate	15385415	1
Caelo	Estradiol hemihydrate	1705018-01	3
Fagron	Estradiol hemihydrate	16H04-B01-334200	1
Caelo	Estradiol hemihydrate	18082101	1
Euro OTC	Estradiol hemihydrate	1802013-01	2
Caelo	Estradiol hemihydrate	18082104	1
Fagron	Estradiol hemihydrate	18F18-B01-351790	1
Euro OTC	Estradiol hemihydrate	1808032-01	3

- 78 795 spectra from 565 *Apo-Ident* customers from a total of 26 067 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	499	0	73 997
Type B	0	1499	36	125 357
Type C	0	132	2	78 795

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.7976 %)
Type B	100.0000 % (> 99.9901 %)	97.6547 % (> 97.4593 %)
Type C	100.0000 % (> 99.9817 %)	98.5075 % (> 96.2687 %)

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

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

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21847	21847	0.00	41.39
21291	21945	4.02	41.10
21667	21945	1.37	39.98
21945	21945	0.00	40.54
22307	22307	0.00	41.81
22913	22913	0.00	40.17
23184	21945	3.82	42.28
21302	21302	0.00	42.43
21508	21508	0.00	45.28

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Estradiol valerate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20330-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Estradiol valerate; Estradioli valeras

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Estradiol valerate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Estradiol valerate	12D18-N02	20651	40	20120426
Fagron	Estradiol valerate	12D18-N02	21266	40	20120118
Caelo	Estradiol valerate	13264001	21411	40	1410503
Caelo	Estradiol valerate	13264001	21416	60	1510624
Caelo	Estradiol valerate	13264001	21424	40	1410503

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Estradiol valerate	14E26-B02-294846	21646	40	20140616
Caelo	Estradiol valerate	15194802	21989	40	20150708
Caelo	Estradiol valerate	163277	23056	40	20161221*
Caelo	Estradiol valerate	13264001	21411SI	30	1410503
Caelo	Estradiol valerate	13264001	21416SI	30	1510624
Caelo	Estradiol valerate	15194802	21989SI	20	20150708
Caelo	Estradiol valerate	163277	23056SI	40	20161221*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 12 reference samples from the substance/substance group *Estradiol valerate*. These samples are listed above in the [calibration samples](#) section.
- 74 036 spectra from a total of 1618 batches from further 372 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 [†].

- 507 spectra of 24 reference samples from the substance/substance group *Estradiol valerate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estradiol valerate	13264001	21411 [†]	20
Caelo	Estradiol valerate	13264001	21416 [†]	60
Caelo	Estradiol valerate	13264001	21417	20
Caelo	Estradiol valerate	13264001	21418	20
Caelo	Estradiol valerate	13264001	21419	20
Caelo	Estradiol valerate	13264001	21422	20
Caelo	Estradiol valerate	13264001	21423	20
Caelo	Estradiol valerate	13264001	21424 [†]	20
Caelo	Estradiol valerate	13264001	21425	20
Caelo	Estradiol valerate	13264001	21426	20
Fagron	Estradiol valerate	14E26-B02-294846	21646 [†]	20
Caelo	Estradiol valerate	15194802	21989 [†]	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	Estradiol valerate	180674	24030	40
Caelo	Estradiol valerate	13264001	21411SI [†]	15
Caelo	Estradiol valerate	13264001	21416SI [†]	15
Caelo	Estradiol valerate	13264001	21417SI	14
Caelo	Estradiol valerate	13264001	21418SI	15
Caelo	Estradiol valerate	13264001	21419SI	15
Caelo	Estradiol valerate	13264001	21422SI	17
Caelo	Estradiol valerate	13264001	21423SI	15
Caelo	Estradiol valerate	13264001	21425SI	15
Caelo	Estradiol valerate	13264001	21426SI	16
Caelo	Estradiol valerate	15194802	21989SI [†]	10
Caelo	Estradiol valerate	180674	24030SI	40

- 126 385 spectra from a total of 2785 batches from further 781 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 64 *Apo-Ident* customers from 70 batches from the substance/substance group *Estradiol valerate*.

Supplier	Substance	Batch	Spectra
Fagron	Estradiol valerate	11J13-No9	1
Fagron	Estradiol valerate	11K04-N04	1
Fagron	Estradiol valerate	12D18-N02	3
Caelo	Estradiol valerate	12G05-N09	2
Noweda	Estradiol valerate	12A20-N10	1
Fagron	Estradiol valerate	12K05-N02	2
Fagron	Estradiol valerate	12G05-N09	2
Beiersdorf/AHD	Estradiol valerate	12A20-N10	1
Fagron	Estradiol valerate	11k04-n04	1
Fagron	Estradiol valerate	12A20-N10	2
Fagron	Estradiol valerate	13A07-N11	5
Caelo	Estradiol valerate	test	1
Fagron	Estradiol valerate	82201620	1
Fagron	Estradiol valerate	12G05N09	1
Fagron	Estradiol valerate	13D16-N10	4
Fagron	Estradiol valerate	11G18-N04	1
Caelo	Estradiol valerate	13264003	1
Sanacorp	Estradiol valerate	13264002	1
Bayer Pharma GmbH	Estradiol valerate	82201620	1
Fagron	Estradiol valerate	13G09-N05	5
Fagron	Estradiol valerate	13D16N10	1
Fagron	Estradiol valerate	11J13-N09	1
Fagron	Estradiol valerate	13G09N05	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
Phoenix	Estradiol valerate	13G09-N05	1
Fagron	Estradiol valerate	24052014a	1
Fagron	Estradiol valerate	13g09-n05	1
Fagron	Estradiol valerate	13I13-N02	2
Caelo	Estradiol valerate	13264001	1
Fagron	Estradiol valerate	14E26-B02-294847	1
Fagron	Estradiol valerate	14E26-B02-294845	3
Fagron	Estradiol valerate	14E26-B02-296348	6
Caelo	Estradiol valerate	14E26-B02-294845	1
Caelo	Estradiol valerate	14E26-B02-294844	1
Fagron	Estradiol valerate	14E26-B02-302873	3
Fagron	Estradiol valerate	14E26B02	2
Fagron	Estradiol valerate	15C10-B05-305396	1
Fagron	Estradiol valerate	15C10-B05-305395	1
Fagron	Estradiol valerate	15C10-B05-309186	3
Fagron	Estradiol valerate	15C10-B05	1
Fagron	Estradiol valerate	15C10-B05-308851	5
Caelo	Estradiol valerate	4214U-03259	1
Fagron	Estradiol valerate	15c10-b05-309186	1
Caelo	Estradiol valerate	15C10B05308851	1
Caelo	Estradiol valerate	15194808	1
Caelo	Estradiol valerate	15c10-B05-305396	1
Fagron	Estradiol valerate	15C10-B05-313568	1
Fagron	Estradiol valerate	15C10-B05-314840	3
Fagron	Estradiol valerate	15C10-B05-318405	1
Fagron	Estradiol valerate	15C10-B05314840	1
Fagro	Estradiol valerate	15C10-B05-318405	1
Caelo	Estradiol valerate	15C10-B05-314840	1
Fagron	Estradiol valerate	19c10-b05-318405	1
Caelo	Estradiol valerate	5315A-03259	1
Fragon	Estradiol valerate	15C10-B05-5314840	1
Caelo	Estradiol valerate	15c10-b05-314840	1
Fagron	Estradiol valerate	15C10-B05-321675	4
Caelo	Estradiol valerate	16327702	1
Phönix	Estradiol valerate	15C10-B05-326087	1
Fagron	Estradiol valerate	15C10B05321675	1
Frago/Gehe	Estradiol valerate	15C10-B0508561040	1
Fagron	Estradiol valerate	15C10-B05-326087	1
Hedinger/Noweda	Estradiol valerate	15C10-B05	1
Frago/Noweda	Estradiol valerate	16F09-B01-329621	1
Caelo	Estradiol valerate	16327706	2
Euro OTC	Estradiol valerate	15C10-b05	1
Fagron	Estradiol valerate	15C10B05-326087	1
Frago/Noweda	Estradiol valerate	16F09-B01	2
Fagron	Estradiol valerate	84404140	2
Fagron	Estradiol valerate	16F09-B01-328135	3
GEHE	Estradiol valerate	16F09-B01-332757	1
Caelo	Estradiol valerate	16327709	1
Caelo	Estradiol valerate	16327710	1
Caelo	Estradiol valerate	16327703	1
Frago/Noweda	Estradiol valerate	16F09-B01-332757	1
Fagron	Estradiol valerate	16F09-B01332756	1
Fagron	Estradiol valerate	16F09-B01-332756	2
Caelo	Estradiol valerate	18067402	4
Caelo	Estradiol valerate	16F09-B01-332756	1
Caelo	Estradiol valerate	18062402	1
Caelo	Estradiol valerate	18067405	1
THC/Phönix	Estradiol valerate	18067402	1
Caelo	Estradiol valerate	18067409	1
Caelo	Estradiol valerate	1810013	1

- 78 798 spectra from 565 *Apo-Ident* customers from a total of 26 068 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	460	0	74 036
Type B	0	507	0	126 385
Type C	0	121	10	78 798

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.8166 %)
Type C	100.0000 % (> 99.8817 %)	92.3664 % (> 90.0763 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21411	21411	0.00	36.28
21989	21424	3.02	45.87
21416	21416	0.00	37.56
21266	23056	6.69	53.85
21424	21424	0.00	47.96
21646	21424	5.33	52.79
23056	23056	0.00	55.73
20651	21411	2.46	36.06

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Estriol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20878-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Estriol; Estriolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Estriol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Estriol	12298706	20878	40	20121106
Fagron	Estriol	11J13-N07	21255	40	1412180
Caelo	Estriol	13256001	21390	40	1511155
Euro OTC	Estriol	1507026	21848	40	0000010671
Euro OTC	Estriol	1509042	21939	40	20151009*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Estriol	16D15-B03-322957	22889	40	20160711
Fagron	Estriol	16I19-B01-331468	23172	40	20170301
Euro OTC	Estriol	1703044	23181	40	20170502*
Caelo	Estriol	13256001	21390SI	40	1511155
Euro OTC	Estriol	1507026	21848SI	40	0000010671
Euro OTC	Estriol	1509042	21939SI	40	20151009*
Fagron	Estriol	16D15-B03-322957	22889SI	40	20160711

Validation samples

A total of 280317 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 *Estriol*. These samples are listed above in the [calibration samples](#) section.
- 74016 spectra from a total of 1615 batches from further 372 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 [†].

- 1165 spectra of 38 reference samples from the substance/substance group *Estriol*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Estriol	1310002-01	21292	40
Caelo	Estriol	13256001	21390 [†]	15
Caelo	Estriol	13256001	21391	60
Caelo	Estriol	13256001	21392	20
Caelo	Estriol	13256001	21393	60
Caelo	Estriol	13256001	21394	20
Caelo	Estriol	13256001	21395	20
Caelo	Estriol	13256001	21399	20
Caelo	Estriol	13256001	21400	20
Caelo	Estriol	13256001	21401	20
Caelo	Estriol	13256001	21404	20
Euro OTC	Estriol	1507026	21848 [†]	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	Estriol	1509042	21939 [†]	20
Caelo	Estriol	161382	22633	40
Euro OTC	Estriol	1606044	22711	40
Euro OTC	Estriol	1610035	22850	40
Euro OTC	Estriol	1710022	23731	40
Euro OTC	Estriol	1710030	23733	40
Euro OTC	Estriol	1803011	24073	40
Caelo	Estriol	13256001	21390SI [†]	20
Caelo	Estriol	13256001	21391SI	60
Caelo	Estriol	13256001	21392SI	20
Caelo	Estriol	13256001	21394SI	20
Caelo	Estriol	13256001	21395SI	20
Caelo	Estriol	13256001	21399SI	20
Caelo	Estriol	13256001	21400SI	20
Caelo	Estriol	13256001	21401SI	20
Caelo	Estriol	13256001	21404SI	20
Euro OTC	Estriol	1507026	21848SI [†]	20
Euro OTC	Estriol	1509042	21939SI [†]	20
Caelo	Estriol	161382	22633SI	40
Euro OTC	Estriol	1606044	22711SI	40
Euro OTC	Estriol	1610035	22850SI	40
Fagron	Estriol	16I19-B01-331468	23172SI	30
Euro OTC	Estriol	1703044	23181SI	40
Euro OTC	Estriol	1710022	23731SI	40
Euro OTC	Estriol	1710030	23733SI	40
Euro OTC	Estriol	1803011	24073SI	40

- 125 727 spectra from a total of 2777 batches from further 781 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.

- 256 spectra from 118 *Apo-Ident* customers from 104 batches from the substance/substance group *Estriol*.

Supplier	Substance	Batch	Spectra
Euro OTC	Estriol	1201020-01	1
Caelo	Estriol	11254402	1
Caelo	Estriol	11254410	1
Fagron	Estriol	12F08-N06	1
Caelo	Estriol	12H06N02	1
Noweda	Estriol	11J13-No7	1
Caelo	Estriol	12032503	4
Fagron	Estriol	11J13-N07	3
Fagron	Estriol	12H06-N02	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
Caelo	Estriol	10053206	1
Caelo	Estriol	12032507	5
Noweda	Estriol	12032504	1
Fagron	Estriol	12H06-No2	2
Caelo	Estriol	11254412	1
Caelo	Estriol	12H06-N02	1
Fagron	Estriol	11D13-N11	1
Fagron	Estriol	12A26-N02	2
Fagron	Estriol	12K07-N15	2
Caelo	Estriol	12298704	6
Caelo	Estriol	12298702	2
Caelo	Estriol	12032504	2
Caelo	Estriol	27061303	1
Fagron	Estriol	13C15-N04	4
Fagron	Estriol	81100490	1
Haihang Industry	Estriol	20130824	1
Caesar § Lorenz GmbH	Estriol	12298712	1
Caelo	Estriol	12298707	2
Fagron	Estriol	13D19-N02	1
Caelo	Estriol	13256004	9
Caelo	Estriol	12298706	1
Sanacorp	Estriol	13256004	1
Euro OTC	Estriol	1310002-01	1
Fagron	Estriol	13H28-N01	3
Caelo	Estriol	17042014B	1
VDL	Estriol	13256004	1
Caelo	Estriol	14077901	1
Caelo	Estriol	13256001	1
Fagron	Estriol	14B06-B11-291563	1
Fagron	Estriol	14B06-B11-291565	1
Fagron	Estriol	14B06-B11-294565	1
Caelo	Estriol	14077904	9
Caelo	Estriol	14077903	2
Bombastus	Estriol	5128	1
Fischar/Gehe	Estriol	14H29-B02-298072	3
Fagron	Estriol	14E13-B01-294034	3
Fagron	Estriol	14b06b11291565	1
Euro OTC	Estriol	1403011-01	2
Audor Pharma	Estriol	APL00036940E	2
Gehe 30.12.14	Estriol	14B06-B11-291563	1
Kehr/Apomix	Estriol	14077904	1
Caelo	Estriol	14272101	3
Caelo	Estriol	24031501	1
Caelo	Estriol	1477904	1
NWM CHina	Estriol	ES150304	1
Caelo	Estriol	14272104	4
Audor Pharma	Estriol	APL000036940E	1
Caelo	Estriol	10H30-N06	1
fargon	Estriol	12a26-n02	1
Noweda 19.05.2015	Estriol	14272104	1
Caelo	Estriol	15028901	4
Caesar & Loretz GmbH	Estriol	15028901	1
Euro OTC	Estriol	15028904	1
Caelo	Estriol	1409018-01	1
Caesar & Loretz GmbH	Estriol	15028904	1
Fagron	Estriol	14E13-B01-294033	1
Caelo	Estriol	15028904	7
Caelo	Estriol	15008902	1
Audor Pharma	Estriol	APL00037293	1
Caelo	Estriol	15297804	10

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Supplier	Substance	Batch	Spectra
Caelo	Estriol	14j20-b07	1
Shandong Northwest Manu...	Estriol	ETL160302	1
Euro OTC	Estriol	1409018-01	1
Caesar&Loretz,AHC, 19.0...	Estriol	15297804	1
Caelo	Estriol	15028905	2
Fagron	Estriol	15297804	2
Fagron	Estriol	15A15-B07-312064	1
Shandong Northwest Manu...	Estriol	ETL160419	1
Audor Pharma	Estriol	APL00037293E	1
Euro/Phönix	Estriol	1509042-01	1
Caelo	Estriol	15297805	1
Caelo	Estriol	16053405	2
Ensbona/ Sanacorp	Estriol	16053405	1
Caelo	Estriol	16053408	2
Fagron	Estriol	16D15-B03-323016	2
Euro OTC	Estriol	15A15-B07-314241	1
Gehe	Estriol	16053405	1
Euro OTC	Estriol	1606044-01	2
Fagron	Estriol	15A15-B07-314241	2
Caelo	Estriol	16138204	4
Audor Pharma	Estriol		4
Fagron	Estriol	16D15-B03-323017	1
Caelo	Estriol	16317702	3
Caelo	Estriol	16317701	4
Euro OTC	Estriol	1610035-01	3
Caelo	Estriol	16317703	3
Sanacorp	Estriol	16317701	1
Fagron	Estriol	16I19-B01	1
Sanacorp	Estriol	16317702	1
Caelo	Estriol	17133705	1
Caelo	Estriol	17133704	9
Caelo	Estriol	16/19-B01-331467	1
Caelo	Estriol	17133706	10
Caelo	Estriol	17133703	2
Caelo	Estriol	1733706	1
Fagron	Estriol	16I19-B01-331468	1
Fagron	Estriol	16/19-B01-332862	1
Caelo	Estriol	1713373	1
Euro OTC	Estriol	1710030-01	2
Caelo	Estriol	17133709	6
Kehr	Estriol	17133704	1
Caelo	Estriol	17133710	1
Caelo	Estriol	17348701	7
Fiebig	Estriol	17133711	1
Caelo	Estriol	17133711	1
Caelo	Estriol	17348702	6
Fagron	Estriol	16I9-B01	1
Fagron	Estriol	16/19-B01-340536	1
Fagron	Estriol	16I19-B01-331467	1
Caelo	Estriol	17348707	1
Cealo/GEHE	Estriol	17348702	1
Phönix /euro	Estriol	1803011-01	1
Caelo	Estriol	18247101	1
Fagron	Estriol	16/19-B01-351346	1
Kehr	Estriol	18247101	1

- 78 673 spectra from 565 *Apo-Ident* customers from a total of 26 034 batches from a further 693

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

Validation results

The validation runs checked whether the substance/substance group *Estriol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Estriol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 016
Type B	0	1160	5	125 727
Type C	0	241	15	78 673

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9901 %)	99.5708 % (> 99.3133 %)
Type C	100.0000 % (> 99.8817 %)	94.1406 % (> 92.9688 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
23172	21939	1.97	40.97
23181	23181	0.00	38.44
20878	21939	2.86	36.49
21390	21390	0.00	32.97
21255	21255	0.00	37.99
21848	21848	0.00	36.06
21939	21939	0.00	37.14
22889	23181	2.20	37.78

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Ethacridine lactate monohydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20750-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ethacridine lactate monohydrate; Ethacridini lactas monohydricus

Special notes

When selecting the *Ethacridine lactate monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Ethacridine lactate monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ethacridine lact...	12149507	20750	40	20120619
Fagron	Ethacridine lact...	13I24-N03	21265	40	AR-15-FG-007011-02
Euro OTC	Ethacridine lact...	1206016-02	21636	40	20121019
Fagron	Ethacridine lact...	15A29-B02-306219	22500	40	20150205

Validation samples

A total of 280317 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 *Ethacridine lactate monohydrate*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 6 reference samples from the substance/substance group *Ethacridine lactate monohydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ethacridine lactate monohydr...	1206016-02	21636 [†]	20
Euro OTC	Ethacridine lactate monohydr...	1412034-02	22733	40
Caelo	Ethacridine lactate monohydr...	16273403	23247	40
Caelo	Ethacridine lactate monohydr...	172476	23671	40
Caelo	Ethacridine lactate monohydr...	172476	23798	40
Caelo	Ethacridine lactate monohydr...	183146	24355	40

- 126672 spectra from a total of 2784 batches from further 781 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.

- 156 spectra from 101 *Apo-Ident* customers from 56 batches from the substance/substance group *Ethacridine lactate monohydrate*.

[†]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
Fagron	Ethacridine lactate monohydr...	11/07-N05	1
Caelo	Ethacridine lactate monohydr...	10288702	1
Caelo	Ethacridine lactate monohydr...	11J07-N05	1
Finze	Ethacridine lactate monohydr...	90601	1
Fagron	Ethacridine lactate monohydr...	12A02-N10	1
Phoenix	Ethacridine lactate monohydr...	100201	1
Fagron	Ethacridine lactate monohydr...	12G02-N135-15	1
Dermapharm	Ethacridine lactate monohydr...	100201	1
Caelo	Ethacridine lactate monohydr...	12149507	3
Dermapharm	Ethacridine lactate monohydr...	111201	5
Fagron	Ethacridine lactate monohydr...	12G02-N13	4
Anzag	Ethacridine lactate monohydr...	111201	1
Caelo	Ethacridine lactate monohydr...	12G02-N13	2
Fagron	Ethacridine lactate monohydr...	201205001	2
Euro OTC	Ethacridine lactate monohydr...	2905007V-03	1
Fagron	Ethacridine lactate monohydr...	12/24-N04	2
Phönix	Ethacridine lactate monohydr...	111201	1
Fagron	Ethacridine lactate monohydr...	12J24-N04	1
Fagron	Ethacridine lactate monohydr...	12C30-N07	1
Euro OTC	Ethacridine lactate monohydr...	2905007-01	1
Dermapharm	Ethacridine lactate monohydr...	130201	7
Fagron	Ethacridine lactate monohydr...	13/24-N03	3
Chinosol/Anzag	Ethacridine lactate monohydr...	2112A-02196	1
Caelo	Ethacridine lactate monohydr...	12268407	3
Phonix	Ethacridine lactate monohydr...	13I24-N03	1
Fagron	Ethacridine lactate monohydr...	13I24-N03	6
Gehe	Ethacridine lactate monohydr...	13I24-N03	1
Euro OTC	Ethacridine lactate monohydr...	1206016-02	4
Euro OTC	Ethacridine lactate monohydr...	13/24-N03	1
Dermopharm	Ethacridine lactate monohydr...	130201	1
Fagron	Ethacridine lactate monohydr...	13I24-N03	1
phoenix 18.11.2014	Ethacridine lactate monohydr...	13/24-N03	1
Euro OTC	Ethacridine lactate monohydr...	2905007v-03	1
Euro OTC	Ethacridine lactate monohydr...	1206016-03	6
Chinosol/Anzag	Ethacridine lactate monohydr...	914E-02196	1
Caelo	Ethacridine lactate monohydr...	1206016-03	1
Caelo	Ethacridine lactate monohydr...	15/214/R	1
Fagron	Ethacridine lactate monohydr...	14A15-B04-300493	6
Caelo	Ethacridine lactate monohydr...	141203401	1
Euro OTC	Ethacridine lactate monohydr...	1412034-01	5
Fagron	Ethacridine lactate monohydr...	12324N03	1
Fagron	Ethacridine lactate monohydr...	14A15-B04	1
Caelo	Ethacridine lactate monohydr...	15177603	4
Bombastus	Ethacridine lactate monohydr...	14A15-B04-300493	1
Bombastus	Ethacridine lactate monohydr...	13/24-N03	1
Dermopharm	Ethacridine lactate monohydr...	141101	1
Fagron	Ethacridine lactate monohydr...	13/24-N03	1
Caelo	Ethacridine lactate monohydr...	15177608	1
Ebert & Jacobi 19.07...	Ethacridine lactate monohydr...	141101	2
Caelo	Ethacridine lactate monohydr...	1412034-01	1
Caelo	Ethacridine lactate monohydr...	15438003	4
Caelo	Ethacridine lactate monohydr...	15438007	4
Dermapharm	Ethacridine lactate monohydr...	141101	6
Fagron	Ethacridine lactate monohydr...	16e20-b11-322514	1
AHL	Ethacridine lactate monohydr...	141101	1
Fagron	Ethacridine lactate monohydr...	16E20-B11-322514	5
Caelo	Ethacridine lactate monohydr...	15438009	2
Euro OTC	Ethacridine lactate monohydr...	15438007	1
Caelo	Ethacridine lactate monohydr...	16273403	6
Gehe	Ethacridine lactate monohydr...	141101	1

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Supplier	Substance	Batch	Spectra
Caelo	Ethacridine lactate monohydr...	16272401	1
Caelo	Ethacridine lactate monohydr...	16273411	6
Caelo	Ethacridine lactate monohydr...	16272406	1
Rezepturlager - Verläng...	Ethacridine lactate monohydr...	121/15	1
Euro OTC	Ethacridine lactate monohydr...	1412034-03	2
Caelo	Ethacridine lactate monohydr...	16272410	1
Caelo	Ethacridine lactate monohydr...	16272408	1
Caelo	Ethacridine lactate monohydr...	1627412	1
Caelo	Ethacridine lactate monohydr...	17247605	3
Sanacorp HST	Ethacridine lactate monohydr...	17247605	1
Caelo	Ethacridine lactate monohydr...	17247606	1
Caelo	Ethacridine lactate monohydr...	17332303	1
Caelo	Ethacridine lactate monohydr...	7247805	1
Caelo	Ethacridine lactate monohydr...	17332304	4
Euro OTC	Ethacridine lactate monohydr...	17332304	1
Rezepturlager - Verläng...	Ethacridine lactate monohydr...	220/17	1

- 78 773 spectra from 565 *Apo-Ident* customers from a total of 26 082 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ethacridine lactate monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ethacridine lactate monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	210	10	126 672
Type C	0	133	23	78 773

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	95.4545 % (> 94.0909 %)
Type C	100.0000 % (> 99.8817 %)	85.2564 % (> 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
22500	21265	5.14	30.13
20750	21265	5.30	30.07
21265	21265	0.00	30.66
21636	21265	7.62	29.87

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ethosuximide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 24100-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ethosuximide; Ethosuximidum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ethosuximide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Katwijk Chemi...	Ethosuximide	451717	24100	40	20180509
Katwijk Chemi...	Ethosuximide	451645	24101	40	1807457

Validation samples

A total of 280 317 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 *Ethosuximide*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Ethosuximide*.

Supplier	Substance	Batch	Sample ID	Spectra
Katwijk Chemie BV	Ethosuximide	451644	24102	40

- 126 852 spectra from a total of 2788 batches from further 781 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 *Ethosuximide*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ethosuximide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ethosuximide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	40	0	126 852
Type C	0	0	0	78 929

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
24100	24101	6.39	58.22
24101	24101	0.00	59.09

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ethyl hydrogen fumarate calcium**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21532-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ethyl hydrogen fumarate calcium; Calcii ethylhydrogenfumaras

Special notes

When selecting the *Ethyl hydrogen fumarate calcium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 hydrogen fumarate calcium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ethyl hydrogen f...	13B25-N08	21532	40	1411090
Euro OTC	Ethyl hydrogen f...	1310029-01	21562	40	20131126
Euro OTC	Ethyl hydrogen f...	1306012-01	21641	40	1505456
Euro OTC	Ethyl hydrogen f...	1510005	21938	40	20151030*

Validation samples

A total of 280317 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 *Ethyl hydrogen fumarate calcium*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 5 reference samples from the substance/substance group *Ethyl hydrogen fumarate calcium*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ethyl hydrogen fumarate calc...	13B25-N08	21532 [†]	20
Euro OTC	Ethyl hydrogen fumarate calc...	1310029-01	21562 [†]	20
Euro OTC	Ethyl hydrogen fumarate calc...	1306012-01	21641 [†]	20
Euro OTC	Ethyl hydrogen fumarate calc...	1510005	21938 [†]	20
Euro OTC	Ethyl hydrogen fumarate calc...	1601011	22294	60

- 126752 spectra from a total of 2784 batches from further 781 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*.

- 12 spectra from 4 *Apo-Ident* customers from 1 batches from the substance/substance group *Ethyl hydrogen fumarate calcium*.

Supplier	Substance	Batch	Spectra
Euro OTC	Ethyl hydrogen fumarate calc...	1510005-01	12

- 78 917 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 hydrogen fumarate calcium* can clearly be 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 hydrogen fumarate calcium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	140	0	126 752
Type C	0	12	0	78 917

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.8818 %)	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
21532	21532	0.00	42.96
21562	21641	13.90	43.42
21641	21641	0.00	26.38
21938	21938	0.00	47.01

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ethyl hydrogen fumarate magnesium**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21533-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ethyl hydrogen fumarate magnesium; Magnesii ethylhydrogenofumaras

Special notes

When selecting the *Ethyl hydrogen fumarate magnesium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 hydrogen fumarate magnesium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ethyl hydrogen f...	13G10-N01	21533	40	1411091
Euro OTC	Ethyl hydrogen f...	1510006	21937	40	20151030*
Euro OTC	Ethyl hydrogen f...	1601010	22290	40	20160114*
Euro OTC	Ethyl hydrogen f...	1510006-01	23008	40	AR-18-FG-000547-01

Validation samples

A total of 280317 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 *Ethyl hydrogen fumarate magnesium*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 *Ethyl hydrogen fumarate magnesium*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ethyl hydrogen fumarate magn...	13G10-N01	21533 [†]	20
Euro OTC	Ethyl hydrogen fumarate magn...	1306014-01	21642	60
Euro OTC	Ethyl hydrogen fumarate magn...	1510006	21937 [†]	20
Euro OTC	Ethyl hydrogen fumarate magn...	1601010	22290 [†]	20

- 126772 spectra from a total of 2785 batches from further 781 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*.

- 6 spectra from 3 *Apo-Ident* customers from 1 batches from the substance/substance group *Ethyl hydrogen fumarate magnesium*.

Supplier	Substance	Batch	Spectra
Fagron	Ethyl hydrogen fumarate magn...	14H27-B04-299502	6

- 78 923 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 hydrogen fumarate magnesium* can clearly be 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 hydrogen fumarate magnesium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	92	28	126 772
Type C	0	6	0	78 923

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	76.6667 % (> 74.1667 %)
Type C	100.0000 % (> 99.8819 %)	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
23008	23008	0.00	49.14
21533	21533	0.00	45.43
21937	21937	0.00	39.85
22290	22290	0.00	41.83

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Fampridine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20902-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Fampridine; Fampridinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Fampridine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Fampridine	13G26-N06	20902	40	1402686
Fagron	Fampridine	14D11-B06-293750	21541	40	20140113
Fagron	Fampridine	16D11-B07-318220	22491	40	AR-16-FG-011566-01
Fagron	Fampridine	16E25-B03-324097	22894	40	20160609
Caelo	Fampridine	16276001	22905	40	20161024

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fampridine	16276001	23237	40	20161024
Fagron	Fampridine	17K20-B02-349165	24439	40	20180103
Fagron	Fampridine	17K20-B02-349165	24439SI	40	20180103

Validation samples

A total of 280317 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 *Fampridine*. These samples are listed above in the [calibration samples](#) section.
- 74176 spectra from a total of 1617 batches from further 372 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 6 reference samples from the substance/substance group *Fampridine*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Fampridine	14D11-B06-293750	21541 [†]	20
Caelo	Fampridine	16276001	22881	40
Fagron	Fampridine	16E25-B03-324097	22945	40
Caelo	Fampridine	16276001	23074	40
Caelo	Fampridine	172170	23653	40
Fagron	Fampridine	16E25-B03-324097	22894SI	40

- 126672 spectra from a total of 2785 batches from further 781 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](#).

[†]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.

- 17 spectra from 9 *Apo-Ident* customers from 14 batches from the substance/substance group *Fampridine*.

Supplier	Substance	Batch	Spectra
Fagron	Fampridine	13C07-B02-289395	1
Fagron	Fampridine	14D11-B06-296110	1
Fagron	Fampridine	14D11-B40-301641	1
Fagron	Fampridine	14D11-B40-304961	1
Fagron	Fampridine	16D11-B07	1
Caelo	Fampridine	15350002	1
Caelo	Fampridine	15350001	1
Inresa	Fampridine	220825	1
Caelo	Fampridine	16276002	3
Fagron	Fampridine	17D19-B01-333745	1
Fagron	Fampridine	16/19-Bo4-330727	1
Caelo	Fampridine	17217003	2
Caelo	Fampridine	24111801	1
Fagron	Fampridine	18121801	1

- 78 912 spectra from 565 *Apo-Ident* customers from a total of 26 123 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Fampridine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fampridine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 176
Type B	0	208	12	126 672
Type C	0	17	0	78 912

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9901 %)	94.5455 % (> 93.1818 %)
Type C	100.0000 % (> 99.8817 %)	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
20902	20902	0.00	68.35
21541	20902	3.30	67.47
22491	22491	0.00	70.05
22894	22491	2.10	71.07
22905	22491	15.20	68.56
23237	22491	18.84	69.39
24439	22491	5.66	68.43

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Finasteride (form III)**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20955-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Finasteride (form III); Finasteridum (Form III)

Special notes

When selecting the *Finasteride (form III)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Finasteride (form III)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Finasteride (for...	13I03-N01	20955	40	1411272
Euro OTC	Finasteride (for...	1403016-01	21626	40	1506004
Fagron	Finasteride (for...	14A16-B40-295980	21742	40	20140317
Euro OTC	Finasteride (for...	1403016-02	21750	40	20140505
Euro OTC	Finasteride (for...	1605020	22565	40	20160613*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Finasteride (for...	1610012	22856	40	20161116*
Fagron	Finasteride (for...	14A16-B40-295980	21742SI	30	20140317
Euro OTC	Finasteride (for...	1403016-02	21750SI	36	20140505
Euro OTC	Finasteride (for...	1605020	22565SI	40	20160613*
Euro OTC	Finasteride (for...	1610012	22856SI	33	20161116*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 379 spectra of 10 reference samples from the substance/substance group *Finasteride (form III)*. These samples are listed above in the [calibration samples](#) section.
- 74 117 spectra from a total of 1617 batches from further 372 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 †.

- 441 spectra of 14 reference samples from the substance/substance group *Finasteride (form III)*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Finasteride (form III)	1403016-01	21626†	20
Fagron	Finasteride (form III)	14A16-B40-295980	21742†	20
Euro OTC	Finasteride (form III)	1403016-02	21750†	20
Fagron	Finasteride (form III)	15J15-B02-320084	22594	40
Fagron	Finasteride (form III)	15J15-B02-320084	22595	40
Euro OTC	Finasteride (form III)	1704004	23151	40
Euro OTC	Finasteride (form III)	1804010	24129	40
Euro OTC	Finasteride (form III)	1809019	24342	40
Fagron	Finasteride (form III)	14A16-B40-295980	21742SI†	15
Euro OTC	Finasteride (form III)	1403016-02	21750SI†	15
Fagron	Finasteride (form III)	15J15-B02-320084	22594SI	40
Fagron	Finasteride (form III)	15J15-B02-320084	22595SI	40
Euro OTC	Finasteride (form III)	1804010	24129SI	40
Euro OTC	Finasteride (form III)	1809019	24342SI	31

*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.

- 126 451 spectra from a total of 2782 batches from further 781 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 5 *Apo-Ident* customers from 12 batches from the substance/substance group *Finasteride (form III)*.

Supplier	Substance	Batch	Spectra
Fagron	Finasteride (form III)	17011303	1
Fagron	Finasteride (form III)	14111305	1
Fagron	Finasteride (form III)	13I03-N01	2
Fagron	Finasteride (form III)	14L23-B02-306981	1
Euro OTC	Finasteride (form III)	1403016-02	1
Euro OTC	Finasteride (form III)	1411008-01	1
Shandong Northwest Manu...	Finasteride (form III)	FNA160604	1
Fagron	Finasteride (form III)	19041707	1
Euro OTC	Finasteride (form III)	1610012-01	1
Euro OTC	Finasteride (form III)	1704004-01	4
Euro OTC	Finasteride (form III)	C1012/116010	1
Euro OTC	Finasteride (form III)	1804010-01	1

- 78 913 spectra from 565 *Apo-Ident* customers from a total of 26 125 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	379	0	74 117
Type B	0	441	0	126 451
Type C	0	16	0	78 913

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

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.4169 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.6395 %)
Type C	100.0000 % (> 99.8817 %)	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
21742	21626	14.20	60.52
21750	21626	12.69	58.67
21626	21626	0.00	55.39
22565	22565	0.00	57.93
22856	22856	0.00	57.85
20955	20955	0.00	54.21

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Fluocinolonacetonid, micronized
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	21031-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fluocinolonacetonid, micronized; Fluocinoloni acetamidum micron.

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Fluocinolonacetonid, micronized*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Fluocinolonaceto...	2804013E-01	21031	60	1404008
Euro OTC	Fluocinolonaceto...	2804013E-01	21077	60	20121206
Caelo	Fluocinolonaceto...	12035003	21756	40	20120321
Euro OTC	Fluocinolonaceto...	2804013E-01	21822	40	20121206
Fagron	Fluocinolonaceto...	14L19-B04-307101	22267	30	20150219

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fluocinolonaceto...	162281	22637	40	20160907*
Caelo	Fluocinolonaceto...	12035003	21756SI	33	20120321
Euro OTC	Fluocinolonaceto...	2804013E-01	21822SI	40	20121206
Fagron	Fluocinolonaceto...	14L19-B04-307101	22267SI	30	20150219
Caelo	Fluocinolonaceto...	162281	22637SI	30	20160907*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 403 spectra of 10 reference samples from the substance/substance group *Fluocinolonacetoneid, micronized*. These samples are listed above in the [calibration samples](#) section.
- 74 093 spectra from a total of 1619 batches from further 372 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 [†].

- 323 spectra of 12 reference samples from the substance/substance group *Fluocinolonacetoneid, micronized*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fluocinolonacetoneid, microni...	12035003	21756 [†]	20
Euro OTC	Fluocinolonacetoneid, microni...	2804013E-01	21822 [†]	20
Euro OTC	Fluocinolonacetoneid, microni...	2804013E-01	21823	60
Fagron	Fluocinolonacetoneid, microni...	14L19-B04-307101	22267 [†]	15
Fagron	Fluocinolonacetoneid, microni...	14L19-B04-307101	23080	40
Caelo	Fluocinolonacetoneid, microni...	172130	23674	40
Caelo	Fluocinolonacetoneid, microni...	12035003	21756SI [†]	15
Euro OTC	Fluocinolonacetoneid, microni...	2804013E-01	21822SI [†]	20
Euro OTC	Fluocinolonacetoneid, microni...	2804013E-01	21823SI	46
Fagron	Fluocinolonacetoneid, microni...	14L19-B04-307101	22267SI [†]	15
Fagron	Fluocinolonacetoneid, microni...	14L19-B04-307101	23080SI	20
Caelo	Fluocinolonacetoneid, microni...	172130	23674SI	12

*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*).

- 126 569 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 20 spectra from 11 *Apo-Ident* customers from 16 batches from the substance/substance group *Fluocinolonacetonid, micronized*.

Supplier	Substance	Batch	Spectra
Fagron	Fluocinolonacetonid, microni...	13E22-N10	1
Caelo	Fluocinolonacetonid, microni...	12035003	1
Euro OTC	Fluocinolonacetonid, microni...	2804013E-01	1
Caelo	Fluocinolonacetonid, microni...	2804013V-03	1
Fagron	Fluocinolonacetonid, microni...	13L30-B35-295489	1
Fagron	Fluocinolonacetonid, microni...	14L19-B04-615699	1
Fargon/Noweda	Fluocinolonacetonid, microni...	13L13-B35	1
Fagron	Fluocinolonacetonid, microni...	14L19-B04	4
Fagron	Fluocinolonacetonid, microni...	13L30B35295489	1
Fagron	Fluocinolonacetonid, microni...	14L19-B04-317248	1
Euro OTC	Fluocinolonacetonid, microni...	1408022-02	2
Fargon/Kehr	Fluocinolonacetonid, microni...	14L-19-B04	1
Ichthyol Gesellschaft /...	Fluocinolonacetonid, microni...	14L19-B04-321003	1
Fagro/Noweda	Fluocinolonacetonid, microni...	15K06-B02-336730	1
Eurho	Fluocinolonacetonid, microni...	1408022-04	1
Caelo	Fluocinolonacetonid, microni...	16228108	1

- 78 909 spectra from 565 *Apo-Ident* customers from a total of 26 121 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	403	0	74 093
Type B	0	322	1	126 569
Type C	0	14	6	78 909

Hence, these spectra are not independent and are not of *Type B*.

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.5112 %)
Type B	100.0000 % (> 99.9901 %)	99.6904 % (> 98.7616 %)
Type C	100.0000 % (> 99.8817 %)	70.0000 % (> 55.0000 %)

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
21031	21031	0.00	40.54
21756	21031	12.66	37.70
21077	21031	1.66	39.38
21822	21031	13.77	38.18
22267	21031	8.41	41.91
22637	22637	0.00	48.56

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Folic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20370-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Folic acid; Acidum folicum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Folic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Folic acid	12G17-N05	20767	40	20120727
Euro OTC	Folic acid	1401005-01	21288	40	20140131
Euro OTC	Folic acid	1508024	21891	40	20150902*
Euro OTC	Folic acid	1604036	22554	40	20160429*
Euro OTC	Folic acid	1611009	22868	40	20161201*

Validation samples

A total of 280317 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 *Folic acid*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 *Folic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Folic acid	1508024	21891 [†]	20
Euro OTC	Folic acid	1608030	22818	40
Fagron	Folic acid	16C03-B06-322513	23081	40

- 126792 spectra from a total of 2786 batches from further 781 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 10 batches from the substance/substance group *Folic acid*.

*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
Fagron	Folic acid	13G16-N02	4
Fagron	Folic acid	UT11110182	1
Fagron	Folic acid	13A11-N01	1
Euro OTC	Folic acid	1401005-01	1
Euro OTC	Folic acid	1307041-01	1
Fagron	Folic acid	16C03-B06	1
Euro OTC	Folic acid	1611009-01	3
Farmalabor	Folic acid	P1701610	1
Euro OTC	Folic acid	1611009-02	1
Euro OTC	Folic acid	1608030-01	1

- 78 914 spectra from 565 *Apo-Ident* customers from a total of 26 127 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Folic 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 *Folic 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	200	0	74 296
Type B	0	100	0	126 792
Type C	0	15	0	78 914

The substance/substance group *Folic 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 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
20767	22554	3.30	49.63
21288	22554	2.71	49.23
22554	22554	0.00	48.54
21891	21891	0.00	49.49
22868	22868	0.00	48.97

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Fructose**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20074-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Fructose; Fructosum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Fructose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Fructose	1212015-01	21281	40	20130111
Euro OTC	Fructose	1509037	21934	40	20151027*
Euro OTC	Fructose	1512009	22292	40	20160113*
Caelo	Fructose	160667	22481	40	20160425*
Caelo	Fructose	15084311	22490	40	20150316
Euro OTC	Fructose	1701049	22986	40	20170213*

Validation samples

A total of 280 317 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 *Fructose*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 [†].

- 501 spectra of 14 reference samples from the substance/substance group *Fructose*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Fructose	1509037	21934 [†]	20
Euro OTC	Fructose	1512009	22292 [†]	20
Caelo	Fructose	160667	22481 [†]	20
Euro OTC	Fructose	1604024	22547	41
Caelo	Fructose	15271213	22583	40
Euro OTC	Fructose	1607030	22693	40
Fagron	Fructose	16H05-B01-326259	23018	40
Fagron	Fructose	16H05-B01-326259	23082	40
Euro OTC	Fructose	1705002	23391	40
Caelo	Fructose	171439	23422	40
Caelo	Fructose	171439	23673	40
Euro OTC	Fructose	1710034	23901	40
Euro OTC	Fructose	1803040	24087	40
Caelo	Fructose	182916	24364	40

- 126 391 spectra from a total of 2777 batches from further 781 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.

- 445 spectra from 108 *Apo-Ident* customers from 179 batches from the substance/substance group *Fructose*.

Supplier	Substance	Batch	Spectra
Caelo	Fructose	10381011	1
Caelo	Fructose	11258611	1
Caelo	Fructose	10071201	1
Caelo	Fructose	11258627	3
Fagron	Fructose	12A26-N04	1
Caelo	Fructose	11071201	1
Noweda	Fructose	1205022-01	1
Caelo	Fructose	1309213394	1
Fagron	Fructose	12E29-N08	3
Caelo	Fructose	11258628	2
Caelo	Fructose	12132305	5
Caelo	Fructose	11258614	1
Caelo	Fructose	12132309	2
Euro OTC	Fructose	1205022-01	1
Fagron	Fructose	508Q-03394	1
Caelo	Fructose	121e29-n08	1
Caelo	Fructose	12132310	1
Caelo	Fructose	12132314	5
Fagron	Fructose	12H01-N03	1
Euro OTC	Fructose	1201017-01	2
Caelo	Fructose	12H01-N03	1
Fagron	Fructose	13A28-N01	10
Fagron	Fructose	1312A-03394	1
Caelo	Fructose	7051304	1
Caelo	Fructose	13A28-N01	1
Euro OTC	Fructose	1209010-01	1
Caelo	Fructose	12132301	2
Caelo	Fructose	21051303	1
Caelo	Fructose	11I07-N06	1
Caelo	Fructose	12132317	2
Caelo	Fructose	12132313	5
Caelo	Fructose	12132322	2
Fagron	Fructose	12H01-N03	1
Caelo	Fructose	12132325	3
Caelo	Fructose	13098902	3
Caelo	Fructose	3313U-03394	1
Sanacorp	Fructose	K43537721	1
Euro OTC	Fructose	121201-01pzn	1
Euro OTC	Fructose	1212015-01	2
Fagron	Fructose	12K28-N06	2
euroct/gehe	Fructose	1212015-01	1
Caelo	Fructose	12132320	1
Fagron	Fructose	13098906	1
Caelo	Fructose	13098906	4
Euro OTC	Fructose	1307022-01	4
Fagron	Fructose	13E27-N07	2
Lihn/Reformhaus	Fructose	713E-03394	2

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Supplier	Substance	Batch	Spectra
Gatt-Koller / Phoenix	Fructose	3156/0813	1
Fagron	Fructose	13C25-N03	3
Fagron	Fructose	7K21-N12	1
Caelo	Fructose	13098909	1
Phönix	Fructose	12K28-N06	1
Alliance Health 13.02.2...	Fructose	13C25-N03	1
Fagron	Fructose	13J18-B06	2
Fagron	Fructose	1107-N06	1
Caelo	Fructose	13098914	2
Caelo	Fructose	1114A03394	1
Caelo	Fructose	13098911	1
Caelo	Fructose	13098917	3
Caelo	Fructose	31031401	1
Euro OTC	Fructose	1401004-01	4
Caelo	Fructose	13098918	1
Fagron	Fructose	13J18-B06-286899	1
Caelo	Fructose	13098915	1
Caelo	Fructose	10051401	1
Caelo	Fructose	13098922	1
Caelo	Fructose	13098913	4
Euro OTC	Fructose	140100401	1
Caelo	Fructose	14096201	2
GEHE 17.06.2014	Fructose	13098913	1
Fagron	Fructose	13J18-B06-286894	1
Fagron	Fructose	14E01-B04-293505	6
Gatt Koller	Fructose	1544/05141914	1
Phoenix 05.08.2014	Fructose	FR1336122	3
Fagron	Fructose	14E01-B04-29350	1
Caelo	Fructose	20081402	1
Caelo	Fructose	14096205	3
Caelo	Fructose	14096208	2
Caelo	Fructose	14096203	1
Alliance health	Fructose	14E01-B04-293505	2
Caelo	Fructose	13098922	1
Caelo	Fructose	13E27-N07	1
Caelo	Fructose	7111401	1
Fagron	Fructose	13E27-n07	1
Beiersdorf	Fructose	14096208	1
Synopharm	Fructose	202A052	1
Caelo	Fructose	14096219	4
Phoenix 22.12.14	Fructose	1307022-01	1
Phoenix 22.12.14	Fructose	1401004-01	1
Caelo	Fructose	13098904	1
Caelo	Fructose	14096211	1
Fagron	Fructose	14E01-B04	3
Fagron	Fructose	14E01-B04-297098	2
Euro OTC	Fructose	1410009-01	4
Euro OTC	Fructose	141000901	2
Caelo	Fructose	14096207	1
Caelo	Fructose	18021501	1
fragon	Fructose	FR1413072	1
Caelo	Fructose	9031504	1
Caelo	Fructose	14096223	5
Caelo	Fructose	14305203	2
Fagron	Fructose	K43537721	1
Alliance health	Fructose	14K17-B99-300913	3
Fagron	Fructose	14k17-B99	2
Fagron	Fructose	14K17-B99	2
Fagron	Fructose	FR1413072	1
Caelo	Fructose	14096210	1

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Supplier	Substance	Batch	Spectra
Caelo	Fructose	5061503	1
Caelo	Fructose	14096224	2
Fagron	Fructose	FR1443072	8
Fagron	Fructose	14E01B04293506	1
Caelo	Fructose	14305201	1
Caelo	Fructose	14305204	1
Caelo	Fructose	15084305	3
Caelo	Fructose	1081501	1
Caelo	Fructose	15084301	3
Caelo	Fructose	1503045-01	2
Caelo	Fructose	15084308	2
Fagron	Fructose	15A16-B07-305241	1
Fagron	Fructose	14E1-B04-293506	1
Euro OTC	Fructose	1503045-01	7
Fagron	Fructose	15A16-B07	1
Caelo	Fructose	15084312	2
Fagron	Fructose	15A16-B07-303124	1
Caelo	Fructose	15A16-B07	1
Fagron	Fructose	15A16-B07-308950	1
Caelo	Fructose	15A16-B07-305241	1
Caelo	Fructose	14305206	1
Caelo	Fructose	15A16-B07-308950	2
Fagron	Fructose	15121-B01-312701	1
Fagron	Fructose	15/21-B01-312700	1
Caelo	Fructose	15271205	4
Fagron	Fructose	3014Q-03394	1
Caelo	Fructose	1509037-01	2
EuRho	Fructose	1509037-01	4
Euro OTC	Fructose	1512009-01	7
Euro OTC	Fructose	1509037-01	5
Fagron	Fructose	15I21-B01	1
euro//Noweda	Fructose	1509037-01	1
Fagron	Fructose	15/21-B01	1
Fagron	Fructose	1170	1
Jenne	Fructose	15A16-B07	1
Jenne	Fructose	14A16-B07	1
Caelo	Fructose	15271214	2
Fargon	Fructose	15I21-B01-312701	1
Caelo	Fructose	152711201	1
Caelo	Fructose	15084311	1
Euro/Gehe	Fructose	1604024-01	1
Caelo	Fructose	15271213	6
Caelo	Fructose	15271208	1
Ebert & Jacobi 08.08.16	Fructose	1604024-01	1
EuRho/Noweda	Fructose	1604024-01	1
Caelo	Fructose	15271201	1
Caelo	Fructose	15271209	3
Euro OTC	Fructose	1604024-01	3
Euro/Gehe	Fructose	1607030-01	1
apo-ident	Fructose	1607030-01	2
Caelo	Fructose	16066103	3
Euro OTC	Fructose	1607030-01	12
Gehe	Fructose	1607030-01	2
Fagron	Fructose	1521-B01-323021	1
Phoenix	Fructose	15I21-B01	1
Caelo	Fructose	15271215	1
Caelo	Fructose	16066106	7
Fagron	Fructose	15121-B01-323021	1
Fagron	Fructose	516Q-03394	1
Euro OTC	Fructose	AD15190330	1

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Supplier	Substance	Batch	Spectra
Caelo	Fructose	16066107	7
Euro OTC	Fructose	1610033-01	7
Caelo	Fructose	23021708	1
Fagron	Fructose	15I21-B01-323021	5
Caelo	Fructose	1610033-01	2
Fagron	Fructose	326259	1
Fagron	Fructose	15/21-B01-323021	1
Fagron	Fructose	15I21-B01-323020	1
Euro/Noweda	Fructose	1610033-01	2
Caelo	Fructose	17007701	4
Fagron	Fructose	16H05-B01	2
Euro OTC	Fructose	1701049-01	10
Caelo	Fructose	17007702	1
Caelo	Fructose	16066101	2
Euro OTC	Fructose	AD16C91215	1
Caelo	Fructose	170104901	1
Caelo	Fructose	17007708	1
Caelo	Fructose	5081701	1
Fagron	Fructose	16H05-B01-330164	2
Finteler Apotheke	Fructose	16283910	1
Euro OTC	Fructose	1705002-01	4
Caelo	Fructose	16283910	1
Noweda	Fructose	16283910	1
Caelo	Fructose	17007707	2
EuRho	Fructose	1705002-01	1
Caelo	Fructose	1701034-01	1
Caelo	Fructose	2117E-03394	1
Caelo	Fructose	13111705	1
Fagron	Fructose	17007701	1
Fagron	Fructose	1705002-01	1
Caelo	Fructose	1705002-01	1
Euro OTC	Fructose	1710034-01	8
Noweda	Fructose	1710034-01	1
Caelo	Fructose	17143902	3
euro//Noweda	Fructose	1710034-01	1
Noweda	Fructose	17143902	1
Caelo	Fructose	1710034-01	1
EuRho	Fructose	171003401	2
Caelo	Fructose	13041802	1
Caelo	Fructose	17143903	1
Caelo	Fructose	9061804	1
Caelo	Fructose	18061801	1
Euro OTC	Fructose	1803040-01	6
Caelo	Fructose	18082002	2
Caelo	Fructose	17346404	13
Caelo	Fructose	17346405	1
Caelo	Fructose	17346411	2
Caelo	Fructose	31101810	1
Caelo	Fructose	18062005	1
Euro OTC	Fructose	1803040-012	1
Caelo	Fructose	18082005	2
Euro OTC	Fructose	180304001	1
Euro OTC	Fructose	1803040-1	1

- 78 484 spectra from 565 *Apo-Ident* customers from a total of 25 959 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#),

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

Validation results

The validation runs checked whether the substance/substance group *Fructose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fructose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	501	0	126 391
Type C	0	444	1	78 484

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.8024 %)
Type C	100.0000 % (> 99.8817 %)	99.7753 % (> 99.1011 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21281	22481	6.90	38.59
21934	21934	0.00	31.79
22292	22292	0.00	44.55
22481	22481	0.00	41.96
22490	22292	1.52	43.13
22986	22986	0.00	40.73

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Furosemide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20944-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Furosemide; Furosemidum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
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Validation method

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

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

Finally, 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 *Furosemide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Furosemide	13A22-N08	20944	40	1401379
Fagron	Furosemide	14K10-B02-301746	21819	40	20141215
Fagron	Furosemide	17D06-B01-338982	23940	40	20170626

Validation samples

A total of 280317 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 *Furosemide*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 *Furosemide*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Furosemide	14K10-B02-301746	21819 [†]	20
Fagron	Furosemide	16B15-B06-322860	23083	40
Fagron	Furosemide	16B15-B06-322860	23084	40

- 126792 spectra from a total of 2787 batches from further 781 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.

- 21 spectra from 16 *Apo-Ident* customers from 16 batches from the substance/substance group *Furosemide*.

Supplier	Substance	Batch	Spectra
Fagron	Furosemide	12A18-N03	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	Furosemide	11K21-N26	1
Fagron	Furosemide	13A22-N08	4
Fagron	Furosemide	1095H2RI	1
Fagron	Furosemide	12I13-No6	1
Alliance Healthcare/Hed...	Furosemide	12/13-N06	1
Fagron	Furosemide	13E28-B40	2
Fagron	Furosemide	13E28-B40-295538	1
Fagron	Furosemide	13E28-B40-289433	1
IPCA/Noweda	Furosemide	11D29-N08	1
Fagron	Furosemide	15L10-B02-316506	2
Caelo	Furosemide	16B15-B06	1
Fagron	Furosemide	14K10-B02-301746	1
Fagron	Furosemide	16/26-B04-329253	1
Fagron	Furosemide	17d06-b01-335672	1
Fagron	Furosemide	17D06-B01-335672	1

- 78 908 spectra from 565 *Apo-Ident* customers from a total of 26 122 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Furosemide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Furosemide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	21	0	78 908

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 71.4286 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20944	20944	0.00	66.00
21819	20944	6.92	66.01
23940	20944	6.47	64.73

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Fusidic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20780-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Fusidic acid; Acidum fusidicum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Fusidic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Fusidic acid	12G04-N01	20780	40	1401162
Fagron	Fusidic acid	13L13-B01-289513	21733	40	20140113
Fagron	Fusidic acid	14E01-B08-299791	21897	40	20140605

Validation samples

A total of 280 317 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 *Fusidic acid*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Fusidic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Fusidic acid	13L13-B01-289513	21733 [†]	20
Fagron	Fusidic acid	14E01-B08-299791	21897 [†]	20
Fagron	Fusidic acid	15I10-B02-322112	23069	40
Fagron	Fusidic acid	17J06-B02-343675	23943	40

- 126 772 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 26 spectra from 10 *Apo-Ident* customers from 21 batches from the substance/substance group *Fusidic acid*.

Supplier	Substance	Batch	Spectra
Fagron	Fusidic acid	12B23-N03	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	Fusidic acid	13A07-N10	2
Fagron	Fusidic acid	13H19-N05	1
Fagron	Fusidic acid	12G04-No1	1
Fagron	Fusidic acid	13L13-B01-289514	1
Fagron	Fusidic acid	13L13-B01-289513	2
Fagron	Fusidic acid	13L13-B01	1
Fagron	Fusidic acid	4113U-07034	1
Fagron	Fusidic acid	15/10-B02-314192	1
Fagron	Fusidic acid	14E01-B08-299791	3
Fagron	Fusidic acid	15I10-B02	1
Fagron	Fusidic acid	1510-B02319231	1
Ebert 24.08.16	Fusidic acid	1510-B02319452	1
Fagron	Fusidic acid	15I10B02-319231	1
Fagron	Fusidic acid	15I10-B02-326182	1
Fagron	Fusidic acid	17G06-B99-337953	1
Fagron	Fusidic acid	116E-03682	1
Fagron	Fusidic acid	17J06-B02-343677	1
Phoenix/Cealo	Fusidic acid	701714-0003/0918A-07	1
Fagron	Fusidic acid	15/10-b02	2
Fagron	Fusidic acid	FS655	1

- 78 903 spectra from 565 *Apo-Ident* customers from a total of 26 116 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Fusidic 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 *Fusidic 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	120	0	74 376
Type B	0	119	1	126 772
Type C	0	23	3	78 903

The substance/substance group *Fusidic 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 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	99.1667 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	88.4615 % (> 76.9231 %)

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

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

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20780	20780	0.00	26.82
21897	20780	9.19	23.28
21733	20780	2.65	27.05

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Gelatine, white**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20206-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Gelatine, white; Gelatina alba

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Gelatine, white*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Gelatine, white	11334025	20898	40	20111214
Caelo	Gelatine, white	15320504	22499	40	AR-16-FG-014461-01
Caelo	Gelatine, white	15320504	22582	40	AR-16-FG-011564-01

Validation samples

A total of 280 317 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 *Gelatine, white*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1621 batches from further 372 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 [†].

- 85 spectra of 3 reference samples from the substance/substance group *Gelatine, white*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Gelatine, white	15320504	22582 [†]	5
Caelo	Gelatine, white	172772	23792	40
Caelo	Gelatine, white	154419	23793	40

- 126 807 spectra from a total of 2786 batches from further 781 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 17 *Apo-Ident* customers from 16 batches from the substance/substance group *Gelatine, white*.

Supplier	Substance	Batch	Spectra
Caelo	Gelatine, white	4110I-01578	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	Gelatine, white	11019308	1
Caelo	Gelatine, white	12354401	1
Euro OTC	Gelatine, white	1106021-01	2
Caelo	Gelatine, white	11334025	4
Caelo	Gelatine, white	11334020	1
Caelo	Gelatine, white	12354507	3
Caelo	Gelatine, white	14130901	2
Caelo	Gelatine, white	14130912	1
EuRho / 20	Gelatine, white	1106021-01	1
Caelo	Gelatine, white	15084806	1
Caelo	Gelatine, white	15084801	1
Caelo	Gelatine, white	15320502	1
Caelo	Gelatine, white	8031701	1
Caelo	Gelatine, white	1544191916	1
Caelo	Gelatine, white	8051811	1
Caelo	Gelatine, white	15441922	1

- 78 905 spectra from 565 *Apo-Ident* customers from a total of 26 122 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	120	0	74 376
Type B	0	83	2	126 807
Type C	0	23	1	78 905

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	97.6471 % (> 94.1176 %)
Type C	100.0000 % (> 99.8817 %)	95.8333 % (> 83.3333 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22499	22499	0.00	15.52
22582	22582	0.00	15.83
20898	22582	7.37	17.65

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Gentamicin sulfate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20640-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Gentamicin sulfate; Gentamicin sulphate; Gentamicini sulfas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Gentamicin sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Gentamicin sulfate	12B21-N02	20661	40	1411075
Euro OTC	Gentamicin sulfate	1305047-01	21081	30	20130919
Caelo	Gentamicin sulfate	13205003	21580	40	20130723
Euro OTC	Gentamicin sulfate	1305047-03	21582	40	1411076
Fagron	Gentamicin sulfate	14E08-B03-294848	21684	40	20140616

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Gentamicin sulfate	1506016	21837	40	0000010321
Caelo	Gentamicin sulfate	14353504	22604	40	20150119
Euro OTC	Gentamicin sulfate	1610036	22857	40	20161124*
Fagron	Gentamicin sulfate	16B29-B01-328731	23210	40	20160411
Euro OTC	Gentamicin sulfate	1610036-01	23782	40	1804343
Euro OTC	Gentamicin sulfate	1711025	23882	40	20171206*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 430 spectra of 11 reference samples from the substance/substance group *Gentamicin sulfate*. These samples are listed above in the [calibration samples](#) section.
- 74 066 spectra from a total of 1612 batches from further 372 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 †.

- 705 spectra of 17 reference samples from the substance/substance group *Gentamicin sulfate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Gentamicin sulfate	13I19-B05-286565	21578	60
Caelo	Gentamicin sulfate	13205003	21580 [†]	20
Euro OTC	Gentamicin sulfate	1305047-03	21582 [†]	20
Fagron	Gentamicin sulfate	14E08-B03-294848	21684 [†]	20
Euro OTC	Gentamicin sulfate	1305047-03	21697	45
Euro OTC	Gentamicin sulfate	1506016	21837 [†]	20
Euro OTC	Gentamicin sulfate	1604054	22568	40
Caelo	Gentamicin sulfate	170996	23335	40
Euro OTC	Gentamicin sulfate	1808013	24300	40
Caelo	Gentamicin sulfate	183001	24357	40
Fagron	Gentamicin sulfate	13I19-B05-286565	21578SI	60
Caelo	Gentamicin sulfate	13205003	21580SI	60
Fagron	Gentamicin sulfate	14E08-B03-294848	21684SI	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
Euro OTC	Gentamicin sulfate	1506016	21837SI	60
Euro OTC	Gentamicin sulfate	1711025	23882SI	40
Euro OTC	Gentamicin sulfate	1808013	24300SI	40
Caelo	Gentamicin sulfate	183001	24357SI	40

- 126 187 spectra from a total of 2779 batches from further 781 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.

- 754 spectra from 329 *Apo-Ident* customers from 210 batches from the substance/substance group *Gentamicin sulfate*.

Supplier	Substance	Batch	Spectra
Caelo	Gentamicin sulfate	11113303	2
Caelo	Gentamicin sulfate	11113304	1
Euro OTC	Gentamicin sulfate	1106016-01	3
Phönix	Gentamicin sulfate	11113309	1
Euro OTC	Gentamicin sulfate	1106016-02	3
Caelo	Gentamicin sulfate	11113308	4
Fagron	Gentamicin sulfate	12B21-N02	2
Fagron	Gentamicin sulfate	11K21-N17	2
Caelo	Gentamicin sulfate	13091207	1
Caelo	Gentamicin sulfate	12163204	4
Caelo	Gentamicin sulfate	3110806	1
Fagron	Gentamicin sulfate	1221-n02	1
Caelo	Gentamicin sulfate	12163206	1
Euro OTC	Gentamicin sulfate	1106016-03	5
Caelo	Gentamicin sulfate	1710I-01582	1
Fagron	Gentamicin sulfate	11k21-n17	1
Caelo	Gentamicin sulfate	12G04-N16	2
Euro OTC	Gentamicin sulfate	1205021-01	12
Caelo	Gentamicin sulfate	1106016-03	1
Caelo	Gentamicin sulfate	12163207	3
Caelo	Gentamicin sulfate	12146602	8
Caelo	Gentamicin sulfate	12163209	1
Caelo	Gentamicin sulfate	1106016-01	1
Caelo	Gentamicin sulfate	1205021-01	1
Anzag	Gentamicin sulfate	12146602	1
Euro OTC	Gentamicin sulfate	FG11112482	1
Euro OTC	Gentamicin sulfate	2911034-02	1
Caelo	Gentamicin sulfate	12146605	4
Fagron	Gentamicin sulfate	12117-no2	1
phönix	Gentamicin sulfate	1214605	1
Fagron	Gentamicin sulfate	11/09-N10	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
Noweda	Gentamicin sulfate	12146602	1
vdl	Gentamicin sulfate	12146602	1
Phönix	Gentamicin sulfate	12146602	1
Caelo	Gentamicin sulfate	12146604	6
Bombastus	Gentamicin sulfate	1205021-01	1
Fagron	Gentamicin sulfate	12G04-N16	1
Euro OTC	Gentamicin sulfate	1205021-02	17
Fagron	Gentamicin sulfate	12D26-N05	9
Caelo	Gentamicin sulfate	1205021-02	2
Fagron	Gentamicin sulfate	12D6-N05	1
Caelo	Gentamicin sulfate	12146611	11
Caelo	Gentamicin sulfate	12146612	2
Fagron	Gentamicin sulfate	13D24-N05	7
Fujian Fukang Pharmaceu...	Gentamicin sulfate	12G04-N16	2
Gehe	Gentamicin sulfate	12146604	1
Fagron	Gentamicin sulfate	10A29-N06	1
EuRho	Gentamicin sulfate	FG1112482	1
Caelo	Gentamicin sulfate	6082013C	1
Caelo	Gentamicin sulfate	13189603	3
Fargon	Gentamicin sulfate	13D24-N05	1
Caelo	Gentamicin sulfate	13189602	5
Euro OTC	Gentamicin sulfate		1
Fagron	Gentamicin sulfate	1106016-01	1
Caelo	Gentamicin sulfate	13189606	6
Caelo	Gentamicin sulfate	13189607	11
Caelo	Gentamicin sulfate	100017814	1
Caelo	Gentamicin sulfate	73402189	1
Alliance Healthcare	Gentamicin sulfate	12G04-N16	1
Caelo	Gentamicin sulfate	312012	1
Fagron	Gentamicin sulfate	1205021-02	1
Euro OTC	Gentamicin sulfate	1305047-01	9
Caelo	Gentamicin sulfate	13D24-N05	1
Fagron	Gentamicin sulfate	13189607	1
Sanacorp	Gentamicin sulfate	13189607	1
Noweda	Gentamicin sulfate	13189607	1
Euro OTC	Gentamicin sulfate	130504701	1
Caelo	Gentamicin sulfate	13189611	9
Caelo	Gentamicin sulfate	13189608	2
Caelo	Gentamicin sulfate	13I19-B05-286565	1
Gehe am 24.2.14	Gentamicin sulfate	1305047-01	1
Phoenix	Gentamicin sulfate	12D26-N05	1
Fagron	Gentamicin sulfate	13I19-B05-286568	1
Caelo	Gentamicin sulfate	31032014E	1
Fagron	Gentamicin sulfate	13I19-B05	1
Phönix	Gentamicin sulfate	13189611	1
PHOENIX 10.03.2014	Gentamicin sulfate	1305047	1
Caelo	Gentamicin sulfate	13189612	13
Fagron	Gentamicin sulfate	1319-B05-286565	1
Sanacorp	Gentamicin sulfate	13189608	1
Phönix Gotha	Gentamicin sulfate	13189611	1
Fagron	Gentamicin sulfate	13/19-B05-286568	1
Fagron	Gentamicin sulfate	FG1305122	1
Fagron	Gentamicin sulfate	14A30-B04-290861	2
Fagron	Gentamicin sulfate	FG1212646	1
Noweda	Gentamicin sulfate	13189611	1
Fagron	Gentamicin sulfate	13/19-B05	1
EuRho	Gentamicin sulfate	1305047-01	1
Caelo	Gentamicin sulfate	13189613	1
Fagron	Gentamicin sulfate	14A30-B04	3
Noweda	Gentamicin sulfate	13189612	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Gentamicin sulfate	1305047-03	10
Euro OTC	Gentamicin sulfate	130504703	2
Fujian Fukang Pharmacea...	Gentamicin sulfate	14A30-B04-290861	1
Euroo/Phoenix	Gentamicin sulfate	1305047-03	1
Fagron	Gentamicin sulfate	14A30-B04-290858	1
Caelo	Gentamicin sulfate	13189614	2
Caelo	Gentamicin sulfate	13205003	8
Fagron	Gentamicin sulfate	19-B05-286568	1
Phoenix	Gentamicin sulfate	1305047-03	1
Fujian Fukang Pharmaceu...	Gentamicin sulfate	14E08-B03-294848	1
Fagron	Gentamicin sulfate	13F13-N01	1
Anzag	Gentamicin sulfate	1305047-03	1
Caelo	Gentamicin sulfate	1305047-03	3
AHD 29.10.14 EK6,12	Gentamicin sulfate	13205004	1
Caelo	Gentamicin sulfate	7011505	1
Fagron	Gentamicin sulfate	14E08-B03-294848	4
Caelo	Gentamicin sulfate	13205005	14
Fagron	Gentamicin sulfate	14a30-b04-290858	1
Euro OTC	Gentamicin sulfate	1305047	1
Caelo	Gentamicin sulfate	23012015E	1
Sanacorp 06.01.15 EK 6,20	Gentamicin sulfate	1305047-03	1
Sanacorp	Gentamicin sulfate	1305047-03	1
Gehe	Gentamicin sulfate	FG1307194	1
Fargron/AHD	Gentamicin sulfate	12G04-N16	1
Caelo	Gentamicin sulfate	13205004	1
Fagron	Gentamicin sulfate	14E08-B03	2
Euro OTC	Gentamicin sulfate	1407024-01	4
Fagron	Gentamicin sulfate	14E08-B03-294835	2
Caelo	Gentamicin sulfate	13205006	5
Fagron	Gentamicin sulfate	14E08-B03-300619	1
Euro OTC	Gentamicin sulfate	1407024-02	1
Caelo	Gentamicin sulfate	14E08-B03-294841	1
Fagron	Gentamicin sulfate	14e08b03300619	1
Fujian Fukang Pharmacea...	Gentamicin sulfate	14E08-B03-300619	1
Euro OTC	Gentamicin sulfate	1407024-03	2
Euro OTC	Gentamicin sulfate	140702403	1
Anzag	Gentamicin sulfate	1407024-01	1
AHD	Gentamicin sulfate	13205005	2
Caelo	Gentamicin sulfate	14353503	13
Euro OTC	Gentamicin sulfate	1407024	1
Caelo	Gentamicin sulfate	1305047-03(2ma1)	1
Noweda	Gentamicin sulfate	1305005	1
Caelo	Gentamicin sulfate	14353502	2
Caelo	Gentamicin sulfate	13205007	2
Fagron	Gentamicin sulfate	14K28-B06-301951	1
Caelo	Gentamicin sulfate	1435303	1
Fagron	Gentamicin sulfate	14K28-B06	3
Caelo	Gentamicin sulfate	14K28-B06-303646	3
Euro OTC	Gentamicin sulfate	140702404	3
Caelo	Gentamicin sulfate	17081502	1
Fagron	Gentamicin sulfate	14K28-B06-303640	3
Noweda	Gentamicin sulfate	140702404	1
Euro OTC	Gentamicin sulfate	1407024-04	5
Caelo	Gentamicin sulfate	14353504	10
Caesar & Loretz GmbH	Gentamicin sulfate	14353503	1
Fagron	Gentamicin sulfate	14081307	2
Caelo	Gentamicin sulfate	1506016-01	2
Phönix	Gentamicin sulfate	14353502	1
Euro OTC	Gentamicin sulfate	1506016-01	9
Caelo	Gentamicin sulfate	15226502	13

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Supplier	Substance	Batch	Spectra
Bombastus	Gentamicin sulfate	13024-N05	1
Fagron	Gentamicin sulfate	14k28-B06-303640	1
Fagron	Gentamicin sulfate	14E08-B03-294841	1
Euro OTC	Gentamicin sulfate	150601601	1
Fagron	Gentamicin sulfate	14k28-b06-303640	2
Caelo	Gentamicin sulfate	143533504	1
Fagron	Gentamicin sulfate	14K28-B06-303646	5
Caelo	Gentamicin sulfate	15226501	14
Euro OTC	Gentamicin sulfate	1506016-02	23
Caelo	Gentamicin sulfate	143535	1
Caelo	Gentamicin sulfate	1506016-02	2
Caelo	Gentamicin sulfate	20161102-4	1
Caelo	Gentamicin sulfate	14353505	3
Noweda	Gentamicin sulfate	14353504	1
Phoenix	Gentamicin sulfate	15226502	1
Caesar&Loretz GmbH	Gentamicin sulfate	15226501	1
Caelo	Gentamicin sulfate	14K28-B06-303636	1
Euro OTC	Gentamicin sulfate	150601602	2
Fagron	Gentamicin sulfate	15b03-b07-309482	1
Euro OTC	Gentamicin sulfate	4988304	1
Phoenix	Gentamicin sulfate	15226501	1
Caelo	Gentamicin sulfate	15258803	8
Fagron	Gentamicin sulfate	14K28B06303646	2
Caelo	Gentamicin sulfate	15258802	12
Caelo	Gentamicin sulfate	4563125	1
Euro OTC	Gentamicin sulfate	80616-2	1
AHD /Pharmachem Pößneck	Gentamicin sulfate	1506016-02	1
Caelo	Gentamicin sulfate	3714I-01582	1
Fagron	Gentamicin sulfate	15258802	1
Fagron	Gentamicin sulfate	15B03-B07-309482	1
Fagron	Gentamicin sulfate	15B03-B07	1
Fagron	Gentamicin sulfate	15E04-B05-316255	2
Caesar&Loretz GmbH,25.0...	Gentamicin sulfate	15258802	1
Fagron	Gentamicin sulfate	15G29-B09-320305	3
Caelo	Gentamicin sulfate	15B03-B07-309482	1
Yantai Justaware Pharma...	Gentamicin sulfate	14K28-B06	1
Euro OTC	Gentamicin sulfate	1604054-01	14
Caelo	Gentamicin sulfate	15226508	2
Fagron	Gentamicin sulfate	11604054-01	1
Caelo	Gentamicin sulfate	1604054-01	2
Fagron	Gentamicin sulfate	15803-B07-309482	1
Caelo	Gentamicin sulfate	15258810	9
Caelo	Gentamicin sulfate	150320G	1
Caelo	Gentamicin sulfate		3
Audor Pharma	Gentamicin sulfate	1604054-01	1
Caelo	Gentamicin sulfate	15258808	5
Caelo	Gentamicin sulfate	1604054-02	1
Caelo	Gentamicin sulfate	1528802	1
Eurimpharm1	Gentamicin sulfate	1604054-01	1
AHD Lamotte GmbH	Gentamicin sulfate	1604054-02	1
Euro OTC	Gentamicin sulfate	1604054-02	6
PHÖNIX	Gentamicin sulfate	15226514	1
Caelo	Gentamicin sulfate	15226514	4
Fagron	Gentamicin sulfate	15G29-B09-322936	2
Fagron	Gentamicin sulfate	15G29-B09-326632	2
Ichthyol/ALH	Gentamicin sulfate	15258810	1
Caelo	Gentamicin sulfate	15226518	3
Caelo	Gentamicin sulfate	15226513	1
ALH	Gentamicin sulfate	15258813	1
Fagron	Gentamicin sulfate	15G29-B09-326635	1

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Supplier	Substance	Batch	Spectra
Caelo	Gentamicin sulfate	15258813	10
Caelo	Gentamicin sulfate	16119302	1
Sanacorp	Gentamicin sulfate	161003601	1
Caelo	Gentamicin sulfate	15258809	1
Gehe	Gentamicin sulfate	15226517	1
Fagron	Gentamicin sulfate	15G29-B09-322928	1
Caelo	Gentamicin sulfate	14081307	1
Caelo	Gentamicin sulfate	1610036-01	3
Caelo	Gentamicin sulfate	15226517	1
Euro OTC	Gentamicin sulfate	1610036-01	10
Caelo	Gentamicin sulfate	1260417	1
Klosterring	Gentamicin sulfate	15G29-B09	1
Caelo	Gentamicin sulfate	15258815	2
Fagron	Gentamicin sulfate	16B29-B01-328731	2
Caelo	Gentamicin sulfate	15258816	11
Fagron	Gentamicin sulfate	15G29B0932632	1
ALH	Gentamicin sulfate	15258816	1
Phoenix	Gentamicin sulfate	15258816	1
Caelo	Gentamicin sulfate	16B29-B01-328731	1
Eurho/Noweda	Gentamicin sulfate	1604054-02	1
GEHE	Gentamicin sulfate	15258815	1
Caelo	Gentamicin sulfate	15258818	17
Fagron	Gentamicin sulfate	16829-B01-328731	1
GEHE	Gentamicin sulfate	15258808	1
Fagron	Gentamicin sulfate	5214A-01582	1
Euro OTC	Gentamicin sulfate	1610036-015339	1
Caelo	Gentamicin sulfate	15128818	1
Noweda	Gentamicin sulfate	15258818	1
Caelo	Gentamicin sulfate	15258819	4
Caelo	Gentamicin sulfate	20170829/1	1
Caelo	Gentamicin sulfate	15258805	1
Caelo	Gentamicin sulfate	115258818	1
Fagron	Gentamicin sulfate	15258816	1
Sanacorp WE: 28.09.17 ...	Gentamicin sulfate	15258825	1
Caelo	Gentamicin sulfate	1528818	1
Caelo	Gentamicin sulfate	17099603	14
Sanacorp	Gentamicin sulfate	1610036-01	2
Caelo	Gentamicin sulfate	17099601	2
Fagron	Gentamicin sulfate	16B29-B01-328915	1
Fagron	Gentamicin sulfate	17G27-B05	1
Fagron	Gentamicin sulfate	17G27-B05-340121	1
Phoenix	Gentamicin sulfate	16b29-b01-328731	1
Caelo	Gentamicin sulfate	17099604	7
Caelo	Gentamicin sulfate	1709601	1
Euro OTC	Gentamicin sulfate	1711025-01	10
Euro OTC	Gentamicin sulfate	161003601	1
Euro OTC	Gentamicin sulfate	180208G/1711025-01	1
Caelo	Gentamicin sulfate	17099608	6
Caelo	Gentamicin sulfate	161003602	1
Caelo	Gentamicin sulfate	17099606-20180404Ma1	1
Caelo	Gentamicin sulfate	18041804	1
Caelo	Gentamicin sulfate	12011801	1
Caelo	Gentamicin sulfate	17099606	3
Euro OTC	Gentamicin sulfate	1610036-02	5
euro AHD	Gentamicin sulfate	1711025-015586	1
Gehe	Gentamicin sulfate	1711025-01	1
Fagron	Gentamicin sulfate	1711025-01	1
Fagron	Gentamicin sulfate	17099608	1
Caelo	Gentamicin sulfate	17358603	11
	Gentamicin sulfate	1610038-01	1

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Supplier	Substance	Batch	Spectra
Caelo	Gentamicin sulfate	FG1603072	1
Gehe/Euro	Gentamicin sulfate	1610036-02	1
Kehr	Gentamicin sulfate	110036-02	1
Fagron	Gentamicin sulfate	18C12-B02-349025	2
Sanacorp	Gentamicin sulfate	FG1711309	1
Fagron	Gentamicin sulfate	18C12-B02-350	1
Fagron	Gentamicin sulfate	18C12-B02	2
Fagron	Gentamicin sulfate	17099606	1
Euro OTC	Gentamicin sulfate	1604054-03	1
Caelo	Gentamicin sulfate	17358604	1
Apo Ident/ Noweda	Gentamicin sulfate	1711025	1
Fagron	Gentamicin sulfate	18C12-B02-350204	1
Delta Apotheke	Gentamicin sulfate	17358604	1
Caelo	Gentamicin sulfate	17358609	3
Sanacorp	Gentamicin sulfate	17358604	1
Caelo	Gentamicin sulfate	18G06-351916	1
Caelo	Gentamicin sulfate	17358616	3
Sanacorp	Gentamicin sulfate	18C12-B02-349026	1
Caelo	Gentamicin sulfate	17358610	1
Sanacorp	Gentamicin sulfate	17358618	1
Caelo	Gentamicin sulfate	1808013-01	1
Caelo	Gentamicin sulfate	17332419	1

- 78 175 spectra from 565 *Apo-Ident* customers from a total of 25 932 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	430	0	74 066
Type B	0	636	69	126 187
Type C	0	705	49	78 175

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.6047 %)
Type B	100.0000 % (> 99.9901 %)	90.2128 % (> 89.7872 %)
Type C	100.0000 % (> 99.8817 %)	93.5013 % (> 93.1034 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20661	20661	0.00	23.58
21580	21837	5.64	31.98
21582	21582	0.00	25.99
21081	21837	3.40	31.86
23210	21837	4.68	25.53
22604	21837	3.36	27.34
21837	21837	0.00	28.42
23782	23782	0.00	25.81
23882	23882	0.00	24.55
21684	21582	3.29	26.43
22857	22857	0.00	22.10

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Glucose monohydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20031-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Glucose monohydrate; Glucosum monohydricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Glucose monohydr...	11L19-N13	20799	40	20120105
Fagron	Glucose monohydr...	14B04-B01	21274	40	20140304
Euro OTC	Glucose monohydr...	1509006	21905	40	20150914*
Euro OTC	Glucose monohydr...	1601016	22308	40	20160129*
Euro OTC	Glucose monohydr...	1604006	22538	40	20160511*
Euro OTC	Glucose monohydr...	1701002	23006	40	20170213*
Euro OTC	Glucose monohydr...	1807005	24162	40	20180718*

Validation samples

A total of 280 317 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 *Glucose monohydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 216 spectra from a total of 1616 batches from further 372 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 10 reference samples from the substance/substance group *Glucose monohydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Glucose monohydrate	1210034-02	21285	40
Euro OTC	Glucose monohydrate	1509006	21905 [†]	20
Euro OTC	Glucose monohydrate	1601016	22308 [†]	20
Euro OTC	Glucose monohydrate	1607024	22692	40
Caelo	Glucose monohydrate	16184807	23025	40
Caelo	Glucose monohydrate	171368	23304	40
Euro OTC	Glucose monohydrate	1707004	23545	40
Caelo	Glucose monohydrate	173050	23802	40
Euro OTC	Glucose monohydrate	1801009	23897	40
Euro OTC	Glucose monohydrate	1811020	24418	40

- 126 532 spectra from a total of 2779 batches from further 781 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.

- 1139 spectra from 259 *Apo-Ident* customers from 273 batches from the substance/substance group *Glucose monohydrate*.

Supplier	Substance	Batch	Spectra
Caelo	Glucose monohydrate	11082014	1
Caelo	Glucose monohydrate	11082020	1
Eurho/Sanacorp	Glucose monohydrate	1108061-01	2
Caelo	Glucose monohydrate	1134506	1
EuRho	Glucose monohydrate	1108061-01	2
Fagron	Glucose monohydrate	8G31-N09	1
EuRho	Glucose monohydrate	1108061-02	1
Euro OTC	Glucose monohydrate	1406212209	1
Caelo	Glucose monohydrate	11314516	3
Caelo	Glucose monohydrate	11L19-N13	3
Eigenherstellung	Glucose monohydrate	30912HML01	1
Fagron	Glucose monohydrate	E524W	1
Fagron	Glucose monohydrate	11L19-N13	1
Euro OTC	Glucose monohydrate	1204044-02	4
Eigenherstellung	Glucose monohydrate	120912HML02	1
Eigenherstellung	Glucose monohydrate	110912HML01	1
Fagron	Glucose monohydrate	12G30-N01	10
Noweda	Glucose monohydrate	1204044-01	2
Fagron	Glucose monohydrate	151780-0004	1
Euro OTC	Glucose monohydrate	1204044-01	1
EuRho	Glucose monohydrate	2710Q-02209	1
Euro OTC	Glucose monohydrate	E267X	1
Caelo	Glucose monohydrate	11314528	6
Caelo	Glucose monohydrate	12G30-N001	1
Euro OTC	Glucose monohydrate	2023012-1	1
Caelo	Glucose monohydrate	12G30-N01	1
Fagron	Glucose monohydrate	12G30-N01	2
EuRho	Glucose monohydrate	1204044-01	2
Caelo	Glucose monohydrate	11314526	1
Caelo	Glucose monohydrate	12284202	6
Eigenherstellung	Glucose monohydrate	180213HJK01	1
Euro OTC	Glucose monohydrate	1210034-01	9
Caelo	Glucose monohydrate	12284204	2
Fagron	Glucose monohydrate	270313PML01	1
Fagron	Glucose monohydrate	13A25-N01	6
Euro OTC	Glucose monohydrate	2313E-02209	1
Fagron	Glucose monohydrate	12B09-N05	1
Fagron	Glucose monohydrate	13AN01	1
Euro OTC	Glucose monohydrate	1210034-02	9
Fagron	Glucose monohydrate	13A25-No1	1
Noweda	Glucose monohydrate	1210034	1
Euro OTC	Glucose monohydrate	2013U-02209	1
Caelo	Glucose monohydrate	12284206	5
Dextro/Krieger/15.05.13	Glucose monohydrate	13092	1
Fagron	Glucose monohydrate	13A25-N01	2
Fargron	Glucose monohydrate	13A25-N01	1
Dextro Energy GmbH/Sana...	Glucose monohydrate	L1299	1
Fagron	Glucose monohydrate	E571X	1
Roquette Lestrem FR/ No...	Glucose monohydrate	1210034-02	1
Fagron	Glucose monohydrate	13C25-N09	8
Fagron	Glucose monohydrate	13B01-N03	5
Caelo	Glucose monohydrate	12284222	3

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Supplier	Substance	Batch	Spectra
Caelo	Glucose monohydrate	12284219	8
Caelo	Glucose monohydrate	13A25-N01	5
Fagron	Glucose monohydrate	13C25N09	2
Fagron	Glucose monohydrate	13A25-n01	1
Caelo	Glucose monohydrate	12284229	3
Fargon	Glucose monohydrate	13C25-N09	1
Phönix	Glucose monohydrate	1210334-02	1
Fagron	Glucose monohydrate	3413E-02209	1
Eigenherstellung	Glucose monohydrate	110913HJK02	1
Caelo	Glucose monohydrate	11314519	1
Caelo	Glucose monohydrate	13H06-N08	2
Fagron	Glucose monohydrate	13H06-N08	17
Euro OTC	Glucose monohydrate	1305030-01	4
dextro energy / Noweda	Glucose monohydrate	L1299	1
Fagron	Glucose monohydrate	4213Q-02209	1
Caelo	Glucose monohydrate	13157002	2
Caelo	Glucose monohydrate	13157005	12
Euro OTC	Glucose monohydrate	31102013B	1
Euro OTC	Glucose monohydrate	1305030-02	5
Caelo	Glucose monohydrate	12284230	3
Euro OTC	Glucose monohydrate	130503001	1
Dextro Energy	Glucose monohydrate	13171	1
Fragon	Glucose monohydrate	13H06-N08	1
Caelo	Glucose monohydrate	13157008	1
Caelo	Glucose monohydrate	E144C	1
Caelo	Glucose monohydrate	13157007	6
Caelo	Glucose monohydrate	13157004	1
Caelo	Glucose monohydrate	1305030-02	1
Caesar & Lorenz	Glucose monohydrate	13157007	1
Caelo	Glucose monohydrate	13157011	9
Euro OTC	Glucose monohydrate	1305030-02	1
Caelo	Glucose monohydrate	13157012	1
Euro OTC	Glucose monohydrate	1114U2209	1
Fagron	Glucose monohydrate	E144C	1
Euro OTC	Glucose monohydrate	1401019-01	15
Fagron	Glucose monohydrate	14B04-B01	3
Fagron	Glucose monohydrate	14B04-B01-291137	7
Caelo	Glucose monohydrate	13157019	10
Caelo	Glucose monohydrate	12284231	1
Phönix	Glucose monohydrate	1401019-01	1
Caelo	Glucose monohydrate	5051401	1
Fagron	Glucose monohydrate	14B04-B01-291143	2
Caelo	Glucose monohydrate	13157022	1
Gehe	Glucose monohydrate	13157026	2
Euro OTC	Glucose monohydrate	140101902	2
Phönix Gotha	Glucose monohydrate	1401019-01	1
pharma gmbh	Glucose monohydrate	1401019-01	1
Caelo	Glucose monohydrate	13157026	3
Cealo	Glucose monohydrate	13157017	1
Euro OTC	Glucose monohydrate	140101901	1
Gutenberg-Apotheke	Glucose monohydrate	14B04-B01	1
Caelo	Glucose monohydrate	18071402	1
Sanacorp	Glucose monohydrate	12284230	1
Fagron	Glucose monohydrate	14B28-B02-291353	10
Caelo	Glucose monohydrate	14B04-B01-291137	1
Caelo	Glucose monohydrate	14102401	4
Caelo	Glucose monohydrate	13157013	1
Euro OTC	Glucose monohydrate	1103027-01	1
Fagron	Glucose monohydrate	14B28-B02-291354	2
Caelo	Glucose monohydrate	14102411	4

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Supplier	Substance	Batch	Spectra
sanacorp	Glucose monohydrate	13157026	1
Caelo	Glucose monohydrate	14102412	9
Fagron	Glucose monohydrate	14B28-B02	2
Fagron	Glucose monohydrate	13H14-B06-289483	1
Fagron	Glucose monohydrate		1
AHD	Glucose monohydrate	14102407	1
Caelo	Glucose monohydrate	14102407	2
Euro OTC	Glucose monohydrate	1405004-01	16
Caelo	Glucose monohydrate	2101402	1
Fagron	Glucose monohydrate	E0AJ5	1
Caelo	Glucose monohydrate	5092	1
Caelo	Glucose monohydrate	14102418	9
Euro OTC	Glucose monohydrate	140004-01	1
Caelo	Glucose monohydrate	14102416	5
Ph.Eur.8.0	Glucose monohydrate	1401019-02	1
GATT-KOLLER/PHOENIX	Glucose monohydrate	243/02142614	1
GATT-KOLLER/PHOENIX	Glucose monohydrate	243/02141714	1
Dextro Energy GmbH/Gehe	Glucose monohydrate	L4163	2
Caelo	Glucose monohydrate	14102424	1
Euro OTC	Glucose monohydrate	1405004-02	4
Caelo	Glucose monohydrate	14102420	5
Sonnenberg-Apotheke	Glucose monohydrate	140500401	1
Caelo	Glucose monohydrate	14102427	1
Euro OTC	Glucose monohydrate	140500401	1
Caelo	Glucose monohydrate	14102415	1
Euro OTC	Glucose monohydrate	14005004-02	1
Dextro Energy GmbH	Glucose monohydrate	L4036	1
Dextro Energy GmbH/Gehe	Glucose monohydrate	L4164	1
Caelo	Glucose monohydrate	14102421	4
Fagron	Glucose monohydrate	15B01291137	1
Fagron	Glucose monohydrate	14I04-B08	1
Fagron	Glucose monohydrate	14B04-B01-291138	1
Euro OTC	Glucose monohydrate	1108061-01	2
Fagron	Glucose monohydrate	14I04-B08-298602	3
Fagron	Glucose monohydrate	1401019-01	1
Dextro Energy GmbH	Glucose monohydrate	L4273	1
Caelo	Glucose monohydrate	14102430	3
Caelo	Glucose monohydrate	14102430	1
EuRho/Phoenix	Glucose monohydrate	140500401	1
Sanacorp	Glucose monohydrate	14102430	1
Caelo	Glucose monohydrate	14334805	2
Caelo	Glucose monohydrate	14334802	10
Caelo	Glucose monohydrate	14I04-B08	4
Caelo	Glucose monohydrate	11021509	1
Caelo	Glucose monohydrate		2
Noweda 10.02.2015	Glucose monohydrate	14334802	3
Caelo	Glucose monohydrate	14B28-B02-291354	1
Sanacorp	Glucose monohydrate	3/AKD100	1
Bombastus	Glucose monohydrate	14334802	2
Roquette Freres/AHD	Glucose monohydrate	12G30-N01	1
Euro OTC	Glucose monohydrate	1410019-01	6
Dextro Energy GmbH/Gehe	Glucose monohydrate	L4274	1
Caelo	Glucose monohydrate	14334810	5
Euro OTC	Glucose monohydrate	141001901	1
Caelo	Glucose monohydrate	14334806	3
Caelo	Glucose monohydrate	200415PJK01	1
Caelo	Glucose monohydrate	14334808	2
Caelo	Glucose monohydrate	14334807	4
Caelo	Glucose monohydrate	14334811	2
Fagron	Glucose monohydrate	14D30-B06-294678	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Glucose monohydrate	96-01	1
Anzag	Glucose monohydrate	14334810	1
Euro OTC	Glucose monohydrate	1410019-02	4
Caelo/Phönix	Glucose monohydrate	15095601	3
Caelo	Glucose monohydrate	15095601	7
Caelo	Glucose monohydrate	28051507	1
Caelo	Glucose monohydrate	15095602	1
Caelo	Glucose monohydrate	15095605	3
Eigenherstellung	Glucose monohydrate	40615HJK01	1
Phönix Gotha	Glucose monohydrate	1405004-02	1
sana	Glucose monohydrate	15095601	2
Caelo	Glucose monohydrate	1410019-02	1
EuRho/GEHE	Glucose monohydrate	1410019-01	1
Fagron	Glucose monohydrate	14I04-B08-298601	1
Caelo	Glucose monohydrate	15095611	3
Fagron	Glucose monohydrate	14I04B8298602	1
Caelo	Glucose monohydrate	1204044-01	2
Caelo	Glucose monohydrate	15095612	11
Caelo	Glucose monohydrate	15180005	3
Caelo	Glucose monohydrate	15095606	1
Caelo	Glucose monohydrate	15180001	10
Caelo	Glucose monohydrate	15095603	1
Euro OTC	Glucose monohydrate	1504028-01	14
Euro OTC	Glucose monohydrate	15095601	1
Noweda 30.07.2015	Glucose monohydrate	15095612	1
ACM	Glucose monohydrate	KNC1282J14	1
Fagron	Glucose monohydrate	1521-B06-309508	1
Caelo	Glucose monohydrate	15180003	3
Caelo	Glucose monohydrate	15180002	15
Eigenherstellung	Glucose monohydrate	160915HML01	1
Euro/ Sanacorp	Glucose monohydrate	1504028-01	1
Fagron	Glucose monohydrate	15A21-B06-309508	3
Fagron	Glucose monohydrate	1407-808-307707	1
Euro OTC	Glucose monohydrate	1504028-02	10
Euro OTC	Glucose monohydrate	1210034-03	1
Euro OTC	Glucose monohydrate	1509006-01	18
Caelo	Glucose monohydrate	14334809	1
Caelo	Glucose monohydrate	15180009	1
Caelo	Glucose monohydrate	15180010	5
Caelo	Glucose monohydrate	15180012	15
Caelo	Glucose monohydrate	15180015	7
Caelo	Glucose monohydrate	1518002	1
Caelo	Glucose monohydrate	2315Q-02209NP	1
EuRho	Glucose monohydrate	151780	1
Euro OTC	Glucose monohydrate	15040281	1
Euro OTC	Glucose monohydrate	150900601	1
Euro OTC	Glucose monohydrate	150402801	1
Caesar & Loretz GmbH	Glucose monohydrate	15180013	1
Euro OTC	Glucose monohydrate	1509006-02	4
Caelo	Glucose monohydrate	15180013	2
Euro OTC	Glucose monohydrate	15180010	1
Caelo	Glucose monohydrate	15413304	22
Caelo	Glucose monohydrate	15413401	4
Caelo	Glucose monohydrate	15413402	5
Caeolo/Noweda	Glucose monohydrate	15413301	1
Caelo	Glucose monohydrate	15413302	3
Caelo	Glucose monohydrate	15413304/20160309/6	1
Caelo	Glucose monohydrate	15413410	3
Caesa/Phoenix	Glucose monohydrate	15413304	1
Caelo	Glucose monohydrate	613011-3p	1

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Supplier	Substance	Batch	Spectra
Fagron	Glucose monohydrate	1404-B08-298601	2
Euro OTC	Glucose monohydrate	1601016-01	17
Caelo	Glucose monohydrate	15413409	20
Caelo	Glucose monohydrate	15180016	1
Caelo	Glucose monohydrate	160101	1
Noweda 10.032016	Glucose monohydrate	15413304	2
Fagron	Glucose monohydrate	1509006-01	1
Fagron	Glucose monohydrate	14104-808	1
Euro OTC	Glucose monohydrate	1601016-02	3
Caelo	Glucose monohydrate	16049102	4
Caesar & Loretz GmbH	Glucose monohydrate	15413402	1
Caelo	Glucose monohydrate	15413412	2
Caelo/ Noweda	Glucose monohydrate	15413412	1
Caelo	Glucose monohydrate	15413303	1
Euroo	Glucose monohydrate	1604006-01	1
Euro OTC	Glucose monohydrate	160101601	2
Bombastus	Glucose monohydrate	15413410	1
Caesar & Loretz/Noweda	Glucose monohydrate	16049102	1
Euro OTC	Glucose monohydrate	1509006-1	1
Euro OTC	Glucose monohydrate	20160405-04	1
Caelo	Glucose monohydrate	16049101	13
Fagron	Glucose monohydrate	14104-B08-302707	1
phönix	Glucose monohydrate	16049101	1
Fagron	Glucose monohydrate	1404-B08-298604	1
Caelo	Glucose monohydrate	15413405	3
Euro OTC	Glucose monohydrate	1604006-01	15
Caelo	Glucose monohydrate	16049105	8
Caelo	Glucose monohydrate	16049103	1
Caelo	Glucose monohydrate	1604006-01	1
Alliance	Glucose monohydrate	16049101	1
Euro/Alliance Healthcare	Glucose monohydrate	1604006-01	1
Fagron	Glucose monohydrate	14102420	1
Caelo	Glucose monohydrate	16049104	13
Euro OTC	Glucose monohydrate	1604006-02	22
Caelo	Glucose monohydrate	123456	1
Caelo	Glucose monohydrate	1604104	1
Euro/Noweda	Glucose monohydrate	1604006-02	2
Caelo	Glucose monohydrate	150302G	1
apo-ident	Glucose monohydrate	1604006-02	1
Fagron	Glucose monohydrate	4562135	1
Euro OTC	Glucose monohydrate	1607024-01	14
Caelo	Glucose monohydrate	16184802	2
Caelo	Glucose monohydrate	4616M-02209	1
Caelo	Glucose monohydrate	2316E-02209	1
Beiersdorf/Phönix	Glucose monohydrate	L6209	1
phönix	Glucose monohydrate	16049104	1
Caelo	Glucose monohydrate	16049107	3
Caelo	Glucose monohydrate	16049108	1
Caelo	Glucose monohydrate	16184801	16
Dextro GmbH/Noweda	Glucose monohydrate	L5301	1
Caelo	Glucose monohydrate	1618401	2
Euro OTC	Glucose monohydrate	1607024-02	24
Sanacorp	Glucose monohydrate	16184810	1
Caelo	Glucose monohydrate	16184808	5
Caelo	Glucose monohydrate	16184810	16
Caelo	Glucose monohydrate	16184807	7
Anzag	Glucose monohydrate	16184808	1
Euro OTC	Glucose monohydrate	16040060-01	1
Euro OTC	Glucose monohydrate	160704-01	1
Caeolo/Phönix	Glucose monohydrate	16184810	2

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Supplier	Substance	Batch	Spectra
Euro OTC	Glucose monohydrate	1701002-01	16
Caelo	Glucose monohydrate	17005801	3
Sanacorp,30.03.17, 7,12EUR	Glucose monohydrate	16184810	1
Euro OTC	Glucose monohydrate	16184807	1
Caelo	Glucose monohydrate	16184816	2
Caelo	Glucose monohydrate	17005804	7
ACM	Glucose monohydrate	KNC1164J15	1
Caelo	Glucose monohydrate	2017Q-02209	1
Caelo	Glucose monohydrate	17005803	12
Apotheke im Forum	Glucose monohydrate	17010002-01	1
Caelo	Glucose monohydrate	17005802	6
phönix	Glucose monohydrate	16184816	1
Caelo	Glucose monohydrate	1607024-01	1
Caelo	Glucose monohydrate	17005811	1
Caelo	Glucose monohydrate	170058025312	1
Caelo	Glucose monohydrate	17136802	10
Anzag	Glucose monohydrate	17005804	1
Sanacorp	Glucose monohydrate	1607024-01	1
Caelo	Glucose monohydrate	17005812	2
EuRho/Phoenix	Glucose monohydrate	1604006-01	1
Caelo	Glucose monohydrate	1701002-01	2
Euro OTG/ AHD	Glucose monohydrate	1701002-01	1
Euro OTC	Glucose monohydrate	1707004-01	27
Klosterring	Glucose monohydrate	17136802	1
Euro OTC	Glucose monohydrate	1701002-02	4
Caelo	Glucose monohydrate	1707004-01	2
Caelo	Glucose monohydrate	17005813	2
Caelo	Glucose monohydrate	17136801	10
GEHE	Glucose monohydrate	1707004-01	1
Anzag	Glucose monohydrate	17136805	1
Caelo	Glucose monohydrate	17136805	9
Euro OTC	Glucose monohydrate	170700401	1
Caelo	Glucose monohydrate	170058025458	1
Euro OTC	Glucose monohydrate	170704401	1
Euro OTC	Glucose monohydrate	17136801	1
Euro OTC	Glucose monohydrate	151780	1
Caelo	Glucose monohydrate	170058025517	1
Phoenix/Cealo	Glucose monohydrate	17305004	1
Caelo	Glucose monohydrate	17136804	4
Caelo	Glucose monohydrate	17305004	6
Euro OTC	Glucose monohydrate	1801009-01	22
Caesar & Loretz/ Caesar...	Glucose monohydrate	18030004	1
Fagron	Glucose monohydrate	17136805	1
Caelo	Glucose monohydrate	17305003	5
Caelo	Glucose monohydrate	18030004	5
Caelo	Glucose monohydrate	23051801	1
Euro OTC	Glucose monohydrate	23051802	1
Caelo	Glucose monohydrate	170058025621	1
Caelo	Glucose monohydrate	18030006	1
Caelo	Glucose monohydrate	18030003	1
Caelo	Glucose monohydrate	18030006	1
Caelo	Glucose monohydrate	26061802	1
Caelo	Glucose monohydrate	18101902	2
Sanacorp	Glucose monohydrate	18101903	2
GEHE	Glucose monohydrate	18030003	1
Caelo	Glucose monohydrate	18030005	2
Caelo	Glucose monohydrate	18101903	3
Caelo	Glucose monohydrate	18101901	8
Euro OTG/ AHD	Glucose monohydrate	1801009-01	1
Euro OTC	Glucose monohydrate	E255L	1

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Supplier	Substance	Batch	Spectra
Caelo	Glucose monohydrate	24081801	1
Caelo	Glucose monohydrate	27081801	1
Caelo	Glucose monohydrate	18101907	3
Euro OTC	Glucose monohydrate	1807005-01	3
Caelo	Glucose monohydrate	18214701	2
Euro OTC	Glucose monohydrate	187005-001	1
Euro OTC	Glucose monohydrate	1807005-02	1
Gehe	Glucose monohydrate	18101907	1
Caelo	Glucose monohydrate	18214703	3

- 77 790 spectra from 565 *Apo-Ident* customers from a total of 25 867 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 monohydrate* can clearly be 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 monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 216
Type B	0	360	0	126 532
Type C	0	1139	0	77 790

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 99.4732 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
20799	22538	2.64	33.68
21274	21905	2.73	24.16
21905	21905	0.00	28.63
22308	22308	0.00	26.14
22538	22538	0.00	32.91
23006	23006	0.00	25.21
24162	24162	0.00	18.74

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Glucose, anhydrous**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20982-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Glucose, anhydrous; Glucosum anhydricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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, anhydrous*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glucose, anhydrous	12294514	20982	40	1402475
Caelo	Glucose, anhydrous	14033901	21363	40	20140214
Caelo	Glucose, anhydrous	14142310	21703	30	20140523
Caelo	Glucose, anhydrous	16050501	22586	40	20160317

Validation samples

A total of 280317 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 *Glucose, anhydrous*. These samples are listed above in the [calibration samples](#) section.
- 74346 spectra from a total of 1619 batches from further 372 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 [†].

- 95 spectra of 3 reference samples from the substance/substance group *Glucose, anhydrous*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glucose, anhydrous	14142310	21703 [†]	15
Caelo	Glucose, anhydrous	16157401	23583	40
Caelo	Glucose, anhydrous	180129	23820	40

- 126797 spectra from a total of 2786 batches from further 781 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.

- 396 spectra from 86 *Apo-Ident* customers from 147 batches from the substance/substance group *Glucose, anhydrous*.

[†]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	Glucose, anhydrous	106213393	1
Caelo	Glucose, anhydrous	25061204	1
Caelo	Glucose, anhydrous	208223393	1
Caelo	Glucose, anhydrous	12141706	3
Caelo	Glucose, anhydrous	11358823	1
Caelo	Glucose, anhydrous	16101204	1
Caelo	Glucose, anhydrous	16101205	1
Jenne	Glucose, anhydrous	12141705	1
Caelo	Glucose, anhydrous	712213393	1
Caelo	Glucose, anhydrous	12141715	1
Caelo	Glucose, anhydrous	12141718	3
Caelo	Glucose, anhydrous	1001313393	1
Caelo	Glucose, anhydrous	402313393	2
Caelo	Glucose, anhydrous	12141717	1
Caelo	Glucose, anhydrous	12294510	3
Caelo	Glucose, anhydrous	12294509	2
Caelo	Glucose, anhydrous	12141714	2
Caelo	Glucose, anhydrous	12294505	3
Sanacorp	Glucose, anhydrous	12294509	1
Caelo	Glucose, anhydrous	26041303	1
Caelo	Glucose, anhydrous	12141705	1
Caelo	Glucose, anhydrous	15051301	1
Caelo	Glucose, anhydrous	2013Q-03393	1
Caelo	Glucose, anhydrous	12294515	2
Caelo	Glucose, anhydrous	2513M03393	1
Caesar&loretz,Anzag	Glucose, anhydrous	12294509	1
Caelo	Glucose, anhydrous	13178704	3
Caelo	Glucose, anhydrous	12294517	1
Caelo	Glucose, anhydrous	12294519	1
Caelo	Glucose, anhydrous	12294514	2
Caelo	Glucose, anhydrous	13178702	1
Caelo	Glucose, anhydrous	3513I-03393	1
Caelo	Glucose, anhydrous	13178707	2
Caelo	Glucose, anhydrous	13178711	2
Caelo	Glucose, anhydrous	AKD14	1
Phönix	Glucose, anhydrous	13178701	1
Caelo	Glucose, anhydrous	13178715	4
Caelo	Glucose, anhydrous	4313Q3393	1
Caelo	Glucose, anhydrous	12294509-3425311150	1
Caelo	Glucose, anhydrous	13178716	1
Caelo	Glucose, anhydrous	13178718	1
Caelo	Glucose, anhydrous	47131-03393	1
Caelo	Glucose, anhydrous	1317815	1
Caelo	Glucose, anhydrous	5013I3393	1
Caelo	Glucose, anhydrous	214U-03393	1
Fagron	Glucose, anhydrous	13178716	1
Caelo	Glucose, anhydrous	13329501	3
Caelo	Glucose, anhydrous	13329504	2
Caelo	Glucose, anhydrous	13329512	7
GEHE	Glucose, anhydrous	13178715	1
Caelo	Glucose, anhydrous	1114A03393	1
Anzag	Glucose, anhydrous	13329505	1
Caelo	Glucose, anhydrous	14033902	4
Caelo	Glucose, anhydrous	1614U3393	1
Caelo	Glucose, anhydrous	1914I03393	1
Caelo	Glucose, anhydrous	13329503	3
PHOENIX 30.05.2014	Glucose, anhydrous	14033902	1
Caelo	Glucose, anhydrous	14051401	1
Caelo	Glucose, anhydrous	14033906	5
PHOENIX 30.05.2014	Glucose, anhydrous	13329514	1

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Supplier	Substance	Batch	Spectra
Caelo	Glucose, anhydrous	14033901	2
Caelo	Glucose, anhydrous	14033907	5
GEHE 17.07.2014	Glucose, anhydrous	14033907	1
Caelo	Glucose, anhydrous	5081401	1
Caelo	Glucose, anhydrous	13178701	2
Caelo	Glucose, anhydrous	3214M-03393	1
Fagron	Glucose, anhydrous	14142303	1
Caelo	Glucose, anhydrous	14142301	1
Caelo	Glucose, anhydrous	14033908	2
Caelo	Glucose, anhydrous	23091401	1
Caelo	Glucose, anhydrous	14142303	3
AHD	Glucose, anhydrous	14033908	1
Caelo	Glucose, anhydrous	14142304	1
Caelo	Glucose, anhydrous	14142308	1
Caelo	Glucose, anhydrous	3121402	1
Caelo	Glucose, anhydrous	13178712	1
Caelo	Glucose, anhydrous	14142313	2
Caelo	Glucose, anhydrous	14142310	4
Caelo	Glucose, anhydrous	14142314	3
Gehe 27.11.14	Glucose, anhydrous	14142309	1
Caelo	Glucose, anhydrous	14319302	1
Caelo	Glucose, anhydrous	14319304	6
Caelo	Glucose, anhydrous	6031505	1
Phoenix	Glucose, anhydrous	14142310	1
Gehe Kassel	Glucose, anhydrous	14142313	1
Caelo	Glucose, anhydrous	13041501	1
Caelo	Glucose, anhydrous	14319309	3
Caelo	Glucose, anhydrous	1439304	1
Caelo	Glucose, anhydrous	15095001	8
Apotheke-SiO2-Mischung	Glucose, anhydrous	18/15	1
Caelo	Glucose, anhydrous	4071505	1
Caelo	Glucose, anhydrous	15095004	3
Caelo	Glucose, anhydrous	14319310	2
Caelo	Glucose, anhydrous	15095005	2
Caelo	Glucose, anhydrous	14319308	1
Caelo	Glucose, anhydrous	15148802	6
Caelo	Glucose, anhydrous	15148809	1
Caelo	Glucose, anhydrous	10091503	1
Caelo	Glucose, anhydrous	15148801	4
Caelo	Glucose, anhydrous	15095003	1
Caelo	Glucose, anhydrous	15148810	4
Caelo	Glucose, anhydrous	15148803	1
Apotheke/Defektur Misch...	Glucose, anhydrous		1
Caelo	Glucose, anhydrous	15148807	3
Rondell Apotheke	Glucose, anhydrous	15329003	1
Caelo	Glucose, anhydrous	1415U-03393	1
Caelo	Glucose, anhydrous	15148808	3
Caelo	Glucose, anhydrous	15329001	6
Caesar&Loretz	Glucose, anhydrous	15148808	1
Caelo	Glucose, anhydrous	1509500	3
Caelo	Glucose, anhydrous	15148813	1
Euro OTC	Glucose, anhydrous	15148808	1
Fagron	Glucose, anhydrous	15329005	2
Caelo	Glucose, anhydrous	15329005	4
Caelo	Glucose, anhydrous	15329004	4
Caelo	Glucose, anhydrous	15329006	7
Caelo	Glucose, anhydrous	15329008	1
Caelo	Glucose, anhydrous	16050504	1
Caelo	Glucose, anhydrous	16050501	10
Caelo	Glucose, anhydrous	15329002	2

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Supplier	Substance	Batch	Spectra
Phoenix	Glucose, anhydrous	15329010	2
Phoenix	Glucose, anhydrous	15148801	1
Caelo	Glucose, anhydrous	16050503	15
Caelo	Glucose, anhydrous	16050502	4
Caelo	Glucose, anhydrous	15329010	2
Klenk	Glucose, anhydrous	16050502	1
Caelo	Glucose, anhydrous	1650502	1
Sonnen-Apotheke Wefensl...	Glucose, anhydrous	17/16	1
Phoenix	Glucose, anhydrous	16050503	4
Bombastus	Glucose, anhydrous	160505202	1
Allianc. Healthc. /c	Glucose, anhydrous	16050510	1
Caelo	Glucose, anhydrous	16050510	2
Caelo	Glucose, anhydrous	16157403	22
Caesar & Loretz GmbH	Glucose, anhydrous	16157403	1
Gehe	Glucose, anhydrous	16157403	2
Caelo	Glucose, anhydrous	160308G	1
Sonnen-Apotheke Wefensl...	Glucose, anhydrous	34/16	1
Caelo	Glucose, anhydrous	16157406	15
GEHE	Glucose, anhydrous	16157406	1
Caelo	Glucose, anhydrous	16050507	1
Caelo	Glucose, anhydrous	8031703	1
Phoenix	Glucose, anhydrous	16050501	1
Caelo	Glucose, anhydrous	17041701	1
Caelo	Glucose, anhydrous	16157411	7
Caelo	Glucose, anhydrous	2051701	1
Caelo	Glucose, anhydrous	16328801	9
Caelo	Glucose, anhydrous	1061703	1
Caelo	Glucose, anhydrous	6071717	1
Caelo	Glucose, anhydrous	551616157406	1
GEHE	Glucose, anhydrous	16328801	1
21.03.2017	Glucose, anhydrous	6910499	1
Caelo	Glucose, anhydrous	7091705	1
Caelo	Glucose, anhydrous	16328805	8
Audor Pharma	Glucose, anhydrous	16157402	3
GEHE	Glucose, anhydrous	16328805	1
Caelo	Glucose, anhydrous	18111702	1
Caelo	Glucose, anhydrous	16328803	6
Caelo	Glucose, anhydrous	28111714	1
Caelo	Glucose, anhydrous	16328812	6
Caelo	Glucose, anhydrous	15021801	1
GEHE	Glucose, anhydrous	18012902	2
Caelo	Glucose, anhydrous	16328811	1
Caelo	Glucose, anhydrous	18012902	7
Caelo	Glucose, anhydrous	18012905	2
Caelo	Glucose, anhydrous	12041801	1
Caelo	Glucose, anhydrous	14051802	1
Caelo	Glucose, anhydrous	18012907	5
Phönix/Fagon	Glucose, anhydrous	16328807	1
Caelo	Glucose, anhydrous	16328807	1
Caelo	Glucose, anhydrous	15081831	1
Caelo	Glucose, anhydrous	8091810	1
Caelo	Glucose, anhydrous	18012909	1
Caelo	Glucose, anhydrous	18012912	2
Caelo	Glucose, anhydrous	17111803	1
Caelo	Glucose, anhydrous	2021902	1

- 78 533 spectra from 565 *Apo-Ident* customers from a total of 25 991 batches from a further 693

substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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, anhydrous* can clearly be 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, anhydrous* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 346
Type B	0	95	0	126 797
Type C	0	366	30	78 533

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 93.6842 %)
Type C	100.0000 % (> 99.8817 %)	92.4242 % (> 91.6667 %)

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
22586	20982	3.03	63.47
21363	20982	9.72	63.85
21703	20982	6.20	63.98
20982	20982	0.00	61.50

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Glutamic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20436-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Glutamic acid; Acidum glutaminicum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Glutamic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Glutamic acid	11I30-N02	20840	40	AR-15-FG-010446-02
Euro OTC	Glutamic acid	L1405023-01	21720	40	20140627
Euro OTC	Glutamic acid	1604056	22562	40	20160523*
Euro OTC	Glutamic acid	1604056	24124	40	20180613*

Validation samples

A total of 280 317 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 *Glutamic acid*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1620 batches from further 372 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 *Glutamic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Glutamic acid	L1211001-01	21282	40
Euro OTC	Glutamic acid	L1405023-01	21720 [†]	20
Fagron	Glutamic acid	15G31-B08-311884	23599	40

- 126 792 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Glutamic acid*.

*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
Fagron	Glutamic acid	3031502	1
Euro OTC	Glutamic acid	28071505	1

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Glutamic 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 *Glutamic 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	160	0	74 336
Type B	0	100	0	126 792
Type C	0	2	0	78 927

The substance/substance group *Glutamic 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 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8823 %)	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
22562	22562	0.00	50.94
20840	20840	0.00	49.35
21720	22562	7.70	50.84
24124	24124	0.00	50.30

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Glutamine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 23150-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Glutamine; Glutaminum; L-glutamine

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Glutamine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Glutamine	1702007	23150	40	20170322*
Euro OTC	Glutamine	1706010	23543	40	20170802*

Validation samples

A total of 280 317 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 *Glutamine*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Glutamine*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Glutamine	17E05-B06-334869	23415	40
Fagron	Glutamine	17E05-B06-334869	23416	40
Euro OTC	Glutamine	1802010	23950	40
Euro OTC	Glutamine	1806001	24121	40

- 126 732 spectra from a total of 2786 batches from further 781 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 *Glutamine*.

*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
Euro OTC	Glutamine	1706010-01	1

- 78 928 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Glutamine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glutamine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	160	0	126 732
Type C	0	1	0	78 928

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8830 %)	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
23150	23150	0.00	30.89
23543	23543	0.00	29.83

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Glycine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20823-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Glycine; Glycinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Glycine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Glycine	12G13-N04	20823	40	1401163
Fagron	Glycine	13G09-N03	21276	40	20120711
Euro OTC	Glycine	1402022-01	21534	40	AR-15-FG-005430-01
Caelo	Glycine	13157303	21687	40	20130625
Caelo	Glycine	14147006	21818	40	AR-16-FG-012263-01

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glycine	15262518	23124	40	20150910
Caelo	Glycine	170265	23295	40	20170315*
Caelo	Glycine	173493	23834	40	20180117*

Validation samples

A total of 280 317 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 *Glycine*. These samples are listed above in the [calibration samples](#) section.
- 74 176 spectra from a total of 1615 batches from further 372 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 7 reference samples from the substance/substance group *Glycine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Glycine	1402022-01	21284	40
Euro OTC	Glycine	1402022-01	21534 [†]	20
Caelo	Glycine	13157303	21687 [†]	20
Caelo	Glycine	14147006	21818 [†]	20
Euro OTC	Glycine	1605035	22683	40
Euro OTC	Glycine	1704015	23387	40
Euro OTC	Glycine	1801005	23912	40

- 126 672 spectra from a total of 2783 batches from further 781 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.

- 8 spectra from 4 *Apo-Ident* customers from 7 batches from the substance/substance group *Glycine*.

Supplier	Substance	Batch	Spectra
Caelo	Glycine	14147005	1
Caelo	Glycine	15262502	2
Caelo	Glycine	15262504	1
Caelo	Glycine	15262503	1
Caelo	Glycine	15262518	1
Caelo	Glycine	17026502	1
Euro OTC	Glycine	1801005-01	1

- 78 921 spectra from 565 *Apo-Ident* customers from a total of 26 130 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	306	14	74 176
Type B	0	219	1	126 672
Type C	0	7	1	78 921

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	95.6250 % (> 94.6875 %)
Type B	100.0000 % (> 99.9901 %)	99.5455 % (> 98.1818 %)
Type C	100.0000 % (> 99.8818 %)	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
23295	23295	0.00	155.34
20823	20823	0.00	137.46
21276	20823	9.00	136.72
21818	21818	0.00	145.21
23124	20823	19.55	130.05
21534	21534	0.00	109.73
21687	21534	9.87	114.10
23834	23834	0.00	115.79

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Glycopyrronium bromide
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	23076-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glycopyrronium bromide; Glycopyrronii bromidum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Glycopyrronium bromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Glycopyrronium b...	16E09-B08-331027	23076	40	1707615
Fagron	Glycopyrronium b...	16E09-B08-331027	23077	40	20160530
Fagron	Glycopyrronium b...	18C30-B07-350744	24183	40	20180502

Validation samples

A total of 280 317 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 *Glycopyrronium bromide*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1621 batches from further 372 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 *Glycopyrronium bromide*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Glycopyrronium bromide	17D28-B04-341606	23939	40

- 126 852 spectra from a total of 2788 batches from further 781 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 *Glycopyrronium bromide*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Glycopyrronium bromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glycopyrronium bromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	40	0	126 852
Type C	0	0	0	78 929

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
23076	23076	0.00	42.59
23077	23076	1.25	42.32
24183	23076	1.94	43.15

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Gramicidin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20203-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Gramicidin; Gramicidinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Gramicidin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Gramicidin	13J15-N02	21253	40	AR-15-FG-000813-01
Fagron	Gramicidin	17E09-B02-341211	23744	40	AR-18-FG-008970-02
Fagron	Gramicidin	18A19-B14-350428	24171	40	20180704

Validation samples

A total of 280 317 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 *Gramicidin*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 [†].

- 192 spectra of 4 reference samples from the substance/substance group *Gramicidin*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Gramicidin	14C07-B06-292886	21544	40
Fagron	Gramicidin	15H18-B01-316269	22748	40
Fagron	Gramicidin	13J15-N02	21253SI	60
Fagron	Gramicidin	14C07-B06-292886	21544SI	52

- 126 700 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 7 spectra from 4 *Apo-Ident* customers from 6 batches from the substance/substance group *Gramicidin*.

Supplier	Substance	Batch	Spectra
Fagron	Gramicidin	11F-24-N03	1
Fagron	Gramicidin	B3200266	1
Fagron	Gramicidin	12K22-N12	1
Fagron	Gramicidin	14H06-B03-297614	2

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Supplier	Substance	Batch	Spectra
Fagron	Gramicidin	15C11-B04-306766	1
Fagron	Gramicidin	17E09-B02-341211	1

- 78 922 spectra from 565 *Apo-Ident* customers from a total of 26 131 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Gramicidin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gramicidin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	89	103	126 700
Type C	0	4	3	78 922

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	46.3542 % (> 44.7917 %)
Type C	100.0000 % (> 99.8818 %)	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
21253	21253	0.00	23.43
23744	23744	0.00	23.14
24171	23744	2.40	22.69

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Griseofulvin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20939-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Griseofulvin; Griseofulvinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
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Validation method

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

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

Finally, 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 *Griseofulvin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Griseofulvin	13D19-N03	20939	40	1401419
Fagron	Griseofulvin	14E16-B01-296834	21725	40	20140526
Fagron	Griseofulvin	16F13-B06-330832	23594	40	20160713

Validation samples

A total of 280 317 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 *Griseofulvin*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Griseofulvin*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Griseofulvin	14E16-B01-296834	21725 [†]	20
Fagron	Griseofulvin	17L05-B05-345995	23996	40
Fagron	Griseofulvin	18L04_B01-357660	24440	40

- 126 792 spectra from a total of 2786 batches from further 781 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 30 *Apo-Ident* customers from 35 batches from the substance/substance group *Griseofulvin*.

Supplier	Substance	Batch	Spectra
Fagron	Griseofulvin	11J11-N13	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
Sanacorp/ F	Griseofulvin	12B06-N07	1
Caelo	Griseofulvin	100910	1
Fagron	Griseofulvin	12F18-N04	1
Fagron	Griseofulvin	10F03-N12	1
Fagron	Griseofulvin	12D04-N12	1
Fagron	Griseofulvin	13F12-N22	1
Fagron	Griseofulvin	13D19-N03	1
Fagron	Griseofulvin	13L-13B08	1
Fagron	Griseofulvin	130922	2
Fagron	Griseofulvin	13L13-B08-290316	3
Fagron	Griseofulvin	13L13-B08	1
Euro OTC	Griseofulvin	14E16-B01-300367	1
Fagron	Griseofulvin	14E16-B01-300366	3
Phönix Gotha	Griseofulvin	140410	1
Fagron	Griseofulvin	140410	2
Fagron	Griseofulvin	15062015A	1
Fagron	Griseofulvin	15B10-B06-396547	1
Fagron	Griseofulvin	15B10-B06-306547	9
Fagron	Griseofulvin	15810-B06	1
Fagron	Griseofulvin	15B10-B06	1
Fagron	Griseofulvin	15B10-B06-306663	1
Fagron	Griseofulvin	15L03-B04-315624	3
Fagron	Griseofulvin	14E16-B01-300367	1
Bombastus	Griseofulvin	15L03-HH150640	1
Fagron	Griseofulvin	15L03-B315624	1
Fagron	Griseofulvin	16F13-B06-323067	2
Fagron	Griseofulvin	15L03-b04-315624	1
Fagron	Griseofulvin	16F13-B06-323068	2
Fargon GmbH & Co.KG	Griseofulvin	16F13-B06-323067	1
Fagron	Griseofulvin	HH160510	1
Caelo	Griseofulvin	16F13-B06-323068	1
Fagron	Griseofulvin	16f13-b06-326074	1
Fagron	Griseofulvin	16F13-B06	1
Fagron	Griseofulvin	16F13-B06-330832	3
Bombastus	Griseofulvin	16F13-B06-326073	1
Fagron	Griseofulvin	16F13-B06-330833	1
Noweda	Griseofulvin	16F13-B06-330833	1
Sanacorp	Griseofulvin	17L05-B05-345995	1
Fagron	Griseofulvin	16f13-b06-330833	1

- 78 869 spectra from 565 *Apo-Ident* customers from a total of 26 102 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Griseofulvin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Griseofulvin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	54	6	78 869

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	90.0000 % (> 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
20939	20939	0.00	72.57
21725	20939	6.52	74.57
23594	20939	1.19	73.24

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Guaifenesin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20551-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Guaifenesin; Guaifenesinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Guaifenesin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Guaifenesin	1212002-01	21287	40	20121214
Euro OTC	Guaifenesin	1506044	21864	40	20150708*
Euro OTC	Guaifenesin	1605005	22555	40	20160525*
Caelo	Guaifenesin	163333	23051	40	20161221*

Validation samples

A total of 280 317 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 *Guaifenesin*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 8 reference samples from the substance/substance group *Guaifenesin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Guaifenesin	1506044	21864 [†]	20
Euro OTC	Guaifenesin	1701011	22993	40
Euro OTC	Guaifenesin	1706006	23551	40
Caelo	Guaifenesin	172496	23644	40
Euro OTC	Guaifenesin	1710033	23741	40
Euro OTC	Guaifenesin	1802001	23949	40
Euro OTC	Guaifenesin	1804004	24076	40
Euro OTC	Guaifenesin	1809011	24316	40

- 126 592 spectra from a total of 2781 batches from further 781 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.

- 11 spectra from 6 *Apo-Ident* customers from 9 batches from the substance/substance group *Guaifenesin*.

Supplier	Substance	Batch	Spectra
Caelo	Guaifenesin	1212002-01	1
Caelo	Guaifenesin	12277307	1
Phoenix 05.07.2014	Guaifenesin	1402023-01	2
Caelo	Guaifenesin	12277311	1
Caelo	Guaifenesin	15302502	1
Caelo	Guaifenesin	16135507	1
Euro OTC	Guaifenesin	1706006-01	2
Euro OTC	Guaifenesin	1804004-01	1
Caelo	Guaifenesin	15F30-b06-317816	1

- 78 918 spectra from 565 *Apo-Ident* customers from a total of 26 128 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Guaifenesin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Guaifenesin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	300	0	126 592
Type C	0	10	1	78 918

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.8818 %)	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
21287	22555	8.67	50.32
21864	21864	0.00	49.38
22555	22555	0.00	48.04
23051	23051	0.00	49.46

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Heparin sodium**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20638-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Heparin sodium; Heparinum natricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
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Validation method

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

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

Finally, 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 *Heparin sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Heparin sodium	12H30-N07	20798	40	1404230
Euro OTC	Heparin sodium	12050009-03	21294	40	AR-15-FG-007427-02
Euro OTC	Heparin sodium	1605022-01	22804	40	9699
Fagron	Heparin sodium	12L20-B01-317990	22824	40	20130312
Yino Pharma	Heparin sodium	YN01011170904	23979	40	20180411
Yino Pharma	Heparin sodium	YN01011170502	23981	40	20180411
Yino Pharma	Heparin sodium	YN01011170904	24195	40	20180531

Validation samples

A total of 280317 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 *Heparin sodium*. These samples are listed above in the [calibration samples](#) section.
- 74216 spectra from a total of 1617 batches from further 372 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 [†].

- 280 spectra of 7 reference samples from the substance/substance group *Heparin sodium*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Heparin sodium	16I26-B02-332108	23591	40
Yino Pharma	Heparin sodium	YN01011R1170803	23976	40
Yino Pharma	Heparin sodium	YN01011R1170803	23977	40
Yino Pharma	Heparin sodium	YN01011170904	23978	40
Yino Pharma	Heparin sodium	YN01011170502	23980	40
Yino Pharma	Heparin sodium	YN010111805002	24196	40
Yino Pharma	Heparin sodium	YN010121805010	24197	40

- 126612 spectra from a total of 2783 batches from further 781 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 9 *Apo-Ident* customers from 11 batches from the substance/substance group *Heparin sodium*.

Supplier	Substance	Batch	Spectra
Fagron	Heparin sodium	12H30-N07	2
Fagron	Heparin sodium	11190188SH	2
Fagron	Heparin sodium	13G03-N13	3
Fagron	Heparin sodium	14D09-B08-307077	1
Fagron	Heparin sodium	14D09-B08-293944	1
Fagron	Heparin sodium	12G19-B02-313422	1
Fiebig	Heparin sodium	16190116C0	1
Fagron	Heparin sodium	12120-B01-323107	1
Fagron	Heparin sodium	16I26-B02-327885	1
Caelo	Heparin sodium	16I26-B02-327885	1
Euro OTC	Heparin sodium	1605022-02	1
Fagron	Heparin sodium	16I26-B02-332108	1

- 78 913 spectra from 565 *Apo-Ident* customers from a total of 26 126 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Heparin sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Heparin sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 216
Type B	0	280	0	126 612
Type C	0	16	0	78 913

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.8817 %)	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
20798	20798	0.00	50.74
23979	21294	7.94	63.90
23981	21294	13.09	43.82
22804	22804	0.00	56.19
22824	21294	7.27	52.27
24195	22804	8.64	53.25
21294	21294	0.00	61.64

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Histamine dihydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20963-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Histamine dihydrochloride; Histamini dihydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
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Validation method

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

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

Finally, 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 *Histamine dihydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Histamine dihydr...	1111004-02	20963	40	1403674
Fagron	Histamine dihydr...	14G16-B02-299175	21668	80	20140729
Euro OTC	Histamine dihydr...	1506030	21863	40	20150706*

Validation samples

A total of 280317 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 *Histamine dihydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1620 batches from further 372 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 *Histamine dihydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Histamine dihydrochloride	14G16-B02-299175	21668 [†]	20
Euro OTC	Histamine dihydrochloride	1506030	21863 [†]	20
Fagron	Histamine dihydrochloride	15C25-B50-331242	23196	40
Fagron	Histamine dihydrochloride	15C25-B50-331242	23197	40

- 126772 spectra from a total of 2786 batches from further 781 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.

- 42 spectra from 22 *Apo-Ident* customers from 23 batches from the substance/substance group *Histamine dihydrochloride*.

*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	Histamine dihydrochloride	1111004-01	4
Fagron	Histamine dihydrochloride	12E29-N09	3
Fagron	Histamine dihydrochloride	12D02-N16	1
Fagron	Histamine dihydrochloride	11E25-N07	2
Fagron	Histamine dihydrochloride	12K06-N08	7
Euro OTC	Histamine dihydrochloride	1111004-02	1
Fagron	Histamine dihydrochloride	28051305	1
Euro OTC	Histamine dihydrochloride	1104004-03	1
Euro OTC	Histamine dihydrochloride	1305006-01	1
Caelo	Histamine dihydrochloride	1111004-02	1
Euro OTC	Histamine dihydrochloride	111004-02	1
Euro OTC	Histamine dihydrochloride	20021412	1
Fagron	Histamine dihydrochloride	14J06B01299179	1
Caelo	Histamine dihydrochloride	130500601	1
Euro OTC	Histamine dihydrochloride	3031503	1
Euro OTC	Histamine dihydrochloride	1411012-02	3
Sanacop	Histamine dihydrochloride	15C25-B01-306047	1
Euro OTC	Histamine dihydrochloride	1506030-01	3
Fagron	Histamine dihydrochloride	15E08-B06-313037	3
Fagron	Histamine dihydrochloride	454545	1
Merck	Histamine dihydrochloride	Wxhc3407V	1
Fa Roth	Histamine dihydrochloride	47252901	1
Merck	Histamine dihydrochloride	Wxhc3407V	1
Fagron	Histamine dihydrochloride	L17100130-0F-222030	1

- 78 887 spectra from 565 *Apo-Ident* customers from a total of 26 114 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Histamine dihydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Histamine dihydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	120	0	126 772
Type C	0	42	0	78 887

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 85.7143 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20963	20963	0.00	75.96
21668	20963	6.07	75.18
21863	21863	0.00	75.97

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Histidine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 23135-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Histidine; Histidinum; L-histidine

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Histidine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Histidine	1703022	23135	40	20170405*
Fagron	Histidine	15I01-B12-329082	23590	40	20150921

Validation samples

A total of 280 317 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 *Histidine*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Histidine*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Histidine	17F15-B04-343276	23935	40

- 126 852 spectra from a total of 2788 batches from further 781 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 *Histidine*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

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

Validation results

The validation runs checked whether the substance/substance group *Histidine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Histidine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	40	0	126 852
Type C	0	0	0	78 929

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
23135	23135	0.00	107.29
23590	23135	5.49	108.45

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Hyaluronic acid sodium salt**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21036-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hyaluronic acid sodium salt; Natrii Hyaluronas

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Hyaluronic acid sodium salt*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor	Hyaluronic acid ...	AP30101702H	23602	40	1802037

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 40 spectra of 1 reference samples from the substance/substance group *Hyaluronic acid sodium salt*. These samples are listed above in the [calibration samples](#) section.
- 74 456 spectra from a total of 1622 batches from further 372 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 4 reference samples from the substance/substance group *Hyaluronic acid sodium salt*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Hyaluronic acid sodium salt	L1302028-01	21036	40
Euro OTC	Hyaluronic acid sodium salt	L1302028-01	21074	60
Audor Pharma	Hyaluronic acid sodium salt	AP30101404H	22262	60
Caelo	Hyaluronic acid sodium salt	172347	23620	40

- 126 692 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 18 spectra from 9 *Apo-Ident* customers from 12 batches from the substance/substance group *Hyaluronic acid sodium salt*.

Supplier	Substance	Batch	Spectra
Caelo	Hyaluronic acid sodium salt	1263303	1
Audor Pharma	Hyaluronic acid sodium salt	AP30101305H	2
Caelo	Hyaluronic acid sodium salt	14188702	1

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Supplier	Substance	Batch	Spectra
Fagron	Hyaluronic acid sodium salt	L1311012-01	1
Audor Pharma	Hyaluronic acid sodium salt	AP30101404H	2
Calo/AHD	Hyaluronic acid sodium salt	14364704	1
Caelo	Hyaluronic acid sodium salt	14364706	2
Caelo	Hyaluronic acid sodium salt	15204901	1
Euro OTC	Hyaluronic acid sodium salt	L1512025-01	2
Audor Pharma	Hyaluronic acid sodium salt	AP30101505H	1
Caelo	Hyaluronic acid sodium salt	15204903	3
Caelo	Hyaluronic acid sodium salt	16246703	1

- 78 911 spectra from 565 *Apo-Ident* customers from a total of 26 125 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	40	0	74 456
Type B	0	69	131	126 692
Type C	0	6	12	78 911

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9888 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9901 %)	34.5000 % (> 33.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
23602	23602	0.00	25.82

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Hydrochlorothiazide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20323-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hydrochlorothiazide; Hydrochlorothiazidum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Hydrochlorothiazide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Hydrochlorothiaz...	11L01-N02	20888	40	20111209
Caelo	Hydrochlorothiaz...	13008505	21589	40	AR-15-FG-014461-01

Validation samples

A total of 280 317 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 *Hydrochlorothiazide*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Hydrochlorothiazide*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrochlorothiazide	13008505	21589 [†]	20
Caelo	Hydrochlorothiazide	14009701	23116	40
Fagron	Hydrochlorothiazide	16F17-B07-327489	23600	40
Fagron	Hydrochlorothiazide	17L20-B02-345079	23989	40
Caelo	Hydrochlorothiazide	182649	24362	40

- 126 712 spectra from a total of 2784 batches from further 781 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.

- 135 spectra from 88 *Apo-Ident* customers from 56 batches from the substance/substance group *Hydrochlorothiazide*.

[†]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
Fagron	Hydrochlorothiazide	11L01-n02	2
Fagron	Hydrochlorothiazide	11L01-N02	2
Gehe	Hydrochlorothiazide	12E04-N02	1
Fagron	Hydrochlorothiazide	11E04-N10	1
Fagron	Hydrochlorothiazide	11Lo1-No2	1
Caelo	Hydrochlorothiazide	11L01n02	1
Fagron	Hydrochlorothiazide	2002311234	1
Fagron	Hydrochlorothiazide	11G12-N12	1
Fagron	Hydrochlorothiazide	11L01-No2	1
Fagron	Hydrochlorothiazide	12L14-N11	4
Fagron	Hydrochlorothiazide	13C25-N08	6
Fagron	Hydrochlorothiazide	CR0601	1
Fagron	Hydrochlorothiazide	12A03-B40	3
Fagron	Hydrochlorothiazide	12E04-N02	1
Fagron	Hydrochlorothiazide	CQ1108	1
Fagron	Hydrochlorothiazide	12A03-B40-286111	3
Fagron	Hydrochlorothiazide	12A03-B40-286110	1
Caelo	Hydrochlorothiazide	13008507	1
Sanacorp	Hydrochlorothiazide	12A03-B40-26111	1
Fagron	Hydrochlorothiazide	14B10-B01-294558	4
Caelo	Hydrochlorothiazide	14B10-B01-294558	2
Caelo	Hydrochlorothiazide	14009701	17
Fagron	Hydrochlorothiazide	5013Q-03660	1
Caelo	Hydrochlorothiazide	13008509	5
Fagron	Hydrochlorothiazide	14b10-b01-294558	1
Fagron	Hydrochlorothiazide	13008504	1
Fagron	Hydrochlorothiazide	14B10-B01-300822	2
Fagron	Hydrochlorothiazide	14B10-B01-305043	2
Fagron	Hydrochlorothiazide	14B10B01	1
Caelo	Hydrochlorothiazide	14B10-B01-305043	2
Fagron	Hydrochlorothiazide	C01-20150412	1
Fagron	Hydrochlorothiazide	Co1-20150412	1
Caelo	Hydrochlorothiazide	15231002	1
Caelo	Hydrochlorothiazide	15231003	4
Fagron	Hydrochlorothiazide	15E04-B03-309670	4
Fagron	Hydrochlorothiazide	15E04-B03	1
Phoenix	Hydrochlorothiazide	15231003	1
Fagron	Hydrochlorothiazide	15K16-B01-315836	2
Fagron	Hydrochlorothiazide	15K16-B01-319833	8
Fagron	Hydrochlorothiazide	15K16	1
Fagron	Hydrochlorothiazide	15K16-B01	2
Caelo	Hydrochlorothiazide	15231005	1
Caelo	Hydrochlorothiazide	15231008	2
Fagron	Hydrochlorothiazide	16F17-B07-324062	5
Sanacorp	Hydrochlorothiazide	15231008	1
Caelo	Hydrochlorothiazide	16269301	2
Caelo	Hydrochlorothiazide	16F17-B07-327489	1
Caelo	Hydrochlorothiazide	16F17B07327489	1
Fagron	Hydrochlorothiazide	16F17-B07-327489	1
Caelo	Hydrochlorothiazide	16269304	1
Fagron	Hydrochlorothiazide	14B10-B01	2
Caelo	Hydrochlorothiazide	16269307	2
Caelo	Hydrochlorothiazide	15231011	1
Caelo	Hydrochlorothiazide	16F17-B07-324062	1
Noweda	Hydrochlorothiazide	16269307	1
Fagron	Hydrochlorothiazide	16F17-B07	2
Fagron	Hydrochlorothiazide	17H28-B01-340561	1
Caelo	Hydrochlorothiazide	16269309	2
GEHE	Hydrochlorothiazide	18017302	1
Caelo	Hydrochlorothiazide	18017303	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrochlorothiazide	16269313	2
Caelo	Hydrochlorothiazide	18017304	2
Caelo	Hydrochlorothiazide	18017302	1
Caelo	Hydrochlorothiazide	18017305	2
Fagron	Hydrochlorothiazide	17L20-B02-347789	2

- 78 794 spectra from 565 *Apo-Ident* customers from a total of 26 081 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Hydrochlorothiazide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hydrochlorothiazide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	180	0	126 712
Type C	0	115	20	78 794

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	85.1852 % (> 82.9630 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
20888	21589	7.68	19.27
21589	21589	0.00	19.13

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Hydrocortisone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20006-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hydrocortisone; Hydrocortisonum purum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Hydrocortisone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Hydrocortisone	1206018-01	21293	40	20130727
Caelo	Hydrocortisone	13341502	21461	40	20131203
Euro OTC	Hydrocortisone	1509029	21899	40	20151014*
Fagron	Hydrocortisone	16A19-B06-320970	22829	40	20160204
Fagron	Hydrocortisone	16A19-B06-321981	22838	40	1702302

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Hydrocortisone	1611016	22910	40	20161220*
Fagron	Hydrocortisone	16H01-B01-326071	22928	40	20160907
Euro OTC	Hydrocortisone	1509029	21899SI	36	20151014*
Fagron	Hydrocortisone	16A19-B06-320970	22829SI	30	20160204
Fagron	Hydrocortisone	16H01-B01-326071	22928SI	40	20160907

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 386 spectra of 10 reference samples from the substance/substance group *Hydrocortisone*. These samples are listed above in the [calibration samples](#) section.
- 74 110 spectra from a total of 1616 batches from further 372 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 †.

- 754 spectra of 21 reference samples from the substance/substance group *Hydrocortisone*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrocortisone	13341502	21461 [†]	20
Caelo	Hydrocortisone	13341502	21463	60
Euro OTC	Hydrocortisone	1509029	21899 [†]	20
Caelo	Hydrocortisone	160952	22778	40
Fagron	Hydrocortisone	16A19-B06-321981	22837	40
Caelo	Hydrocortisone	171194	23340	20
Caelo	Hydrocortisone	171194	23659	40
Caelo	Hydrocortisone	172566	23840	40
Euro OTC	Hydrocortisone	1802009	23945	40
Caelo	Hydrocortisone	180915	24020	40
Caelo	Hydrocortisone	13341502	21463SI	60
Euro OTC	Hydrocortisone	1509029	21899SI [†]	15
Caelo	Hydrocortisone	160952	22778SI	40
Fagron	Hydrocortisone	16A19-B06-321981	22837SI	30

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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
Fagron	Hydrocortisone	16A19-B06-321981	22838SI	31
Euro OTC	Hydrocortisone	1611016	22910SI	40
Caelo	Hydrocortisone	171194	23340SI	28
Caelo	Hydrocortisone	171194	23659SI	30
Caelo	Hydrocortisone	172566	23840SI	40
Euro OTC	Hydrocortisone	1802009	23945SI	40
Caelo	Hydrocortisone	180915	24020SI	40

- 126 138 spectra from a total of 2780 batches from further 781 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.

- 1196 spectra from 368 *Apo-Ident* customers from 261 batches from the substance/substance group *Hydrocortisone*.

Supplier	Substance	Batch	Spectra
Euro OTC	Hydrocortisone	1107005-02	3
Euro OTC	Hydrocortisone	1107005-01	1
Phönix	Hydrocortisone	11119-N03	1
Euro OTC	Hydrocortisone	1107005-03	6
Fagron	Hydrocortisone	11K18-N01	2
Caelo	Hydrocortisone	11260309	3
Anzag	Hydrocortisone	11260305	1
Caelo	Hydrocortisone	12104301	1
Anzag ek:10.01EUR 18.07.12	Hydrocortisone	1107005-03	1
Caelo	Hydrocortisone	12104306	8
Caelo	Hydrocortisone	11260308	3
Noweda	Hydrocortisone	12104303	1
EuRho	Hydrocortisone	1107005-02	1
Caelo	Hydrocortisone	11273704	1
Anzag	Hydrocortisone	1107005-02	1
Caelo	Hydrocortisone	12104304	6
Fagron	Hydrocortisone	12G19-N01	2
Caelo	Hydrocortisone	12104303	5
Gehe	Hydrocortisone	12104304	3
Caelo	Hydrocortisone	12119304	3
Anzag 14.12.12 ek:10,01	Hydrocortisone	1202032-01	1
Caelo	Hydrocortisone	113I-01719	1
Fagron	Hydrocortisone	12/25-N01	1
Sanacorp	Hydrocortisone	1112030-01	1
Caelo	Hydrocortisone	3912Q-01719	1
Caelo	Hydrocortisone	12104307	16
Caelo	Hydrocortisone	12119303	8
Caelo	Hydrocortisone	11021302	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
Euro OTC	Hydrocortisone	1112030-01	7
Caelo	Hydrocortisone	12104308	6
Anzag	Hydrocortisone	12104307	1
phönix	Hydrocortisone		2
Fagron	Hydrocortisone	12I25-N01	2
Euro OTC	Hydrocortisone	1202032-01	3
Caelo	Hydrocortisone	12167001	6
Caelo	Hydrocortisone	12167007	9
Caelo	Hydrocortisone	12k08-n01	1
Noweda	Hydrocortisone	12167001	1
Euro OTC	Hydrocortisone	4112A-01719	1
Caelo	Hydrocortisone	12104305	1
Caelo	Hydrocortisone	2013U-01719	1
Euro OTC	Hydrocortisone	1204037-01	20
Caelo	Hydrocortisone	12104309	2
xxx	Hydrocortisone	911Q-01719	2
Fagron	Hydrocortisone	5061305	1
Phönix	Hydrocortisone	12167001	2
Phönix	Hydrocortisone	12167010	1
Caelo	Hydrocortisone	13069501	8
A.H. 10.06.13 ek: 10,01EUR	Hydrocortisone	1204037-01	1
Caelo	Hydrocortisone	13069502	5
Caelo	Hydrocortisone	12167010	10
Caelo	Hydrocortisone	120403701	1
Phönix Gotha	Hydrocortisone	12104309	1
Klenk	Hydrocortisone	12167007	1
Caelo	Hydrocortisone	10282208	1
Phönix	Hydrocortisone	1204037-01	1
Caelo	Hydrocortisone	13063501	1
Euro OTC	Hydrocortisone	120403701	3
Euro OTC	Hydrocortisone	1204307-01	1
AHC 02.09.13 EK9,85	Hydrocortisone	1112030-01	1
Caesar & Loretz GmbH	Hydrocortisone	12167010	1
AHD	Hydrocortisone	13069507	1
Caelo	Hydrocortisone	7101301	1
Caelo	Hydrocortisone	1109845	1
Fagron	Hydrocortisone	13H08-B01-285472	1
Caelo	Hydrocortisone	13069506	8
Caelo	Hydrocortisone	21101303	1
Caelo	Hydrocortisone	810911	1
Caelo	Hydrocortisone	12167010-3437311151	1
Caelo	Hydrocortisone	13069507	3
Euro OTC	Hydrocortisone	1206018-01	18
Caelo	Hydrocortisone	13069505	4
Fagron	Hydrocortisone	1204037-01	1
Caelo	Hydrocortisone	13155602	8
Caesar & Loretz GmbH	Hydrocortisone	13069507	1
Gehe	Hydrocortisone	13H08-B01-285471	1
Caesar & Loretz GmbH	Hydrocortisone	13069506	1
Caelo	Hydrocortisone	1306906	1
Gehe	Hydrocortisone	13069510	1
sana corp	Hydrocortisone	13069507	1
Caelo	Hydrocortisone	13069509	2
Caelo	Hydrocortisone	1216707	1
Gehe	Hydrocortisone	13H08-B01-285469	1
Fagron	Hydrocortisone	PH132	1
Fagron	Hydrocortisone	13H08B01285473	1
Caelo	Hydrocortisone	13069510	6
Fagron	Hydrocortisone	12119303	1
Caelo	Hydrocortisone	39/AKD17	1

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Supplier	Substance	Batch	Spectra
Fagron	Hydrocortisone	13K22-B01-288283	1
Caelo	Hydrocortisone	13155603	12
Caelo	Hydrocortisone	13155604	6
Caelo	Hydrocortisone	13155601	7
Sanacorp	Hydrocortisone	13069509	1
Caelo	Hydrocortisone	13341502	10
Caelo	Hydrocortisone	31032014D	1
Fagron	Hydrocortisone	13K22-B01-288284	3
Fagron	Hydrocortisone	120601801	1
Caelo	Hydrocortisone	13155605	3
Phönix	Hydrocortisone	13341504	2
Alliance Health 11.01.2. . .	Hydrocortisone	1315505	1
GEHE 14.04.2014	Hydrocortisone	13069509	1
Fagron	Hydrocortisone	13H08-B01-28571	1
Alliance Health25.04.2014	Hydrocortisone	13341503	3
Caelo	Hydrocortisone	13155611	2
Phönix Gotha	Hydrocortisone	13341502	1
Fagron	Hydrocortisone	19051403	1
Caelo	Hydrocortisone	13155614	3
Gehe	Hydrocortisone	1206018-01	2
Noweda	Hydrocortisone	13155605	1
GEHE 03.05.2014	Hydrocortisone	13155605	1
Caelo	Hydrocortisone	13341504	7
ahd,11,95EUR 10.04.14	Hydrocortisone	13341504-07R07	1
Phoenix	Hydrocortisone	13341504	1
Caelo	Hydrocortisone	13341501	6
Pharmacia&Upjohn/ Phönix	Hydrocortisone	13155614	1
EuRho	Hydrocortisone	1405001-01	3
Caelo	Hydrocortisone	13341509	8
Caelo	Hydrocortisone	13341510	11
Caelo	Hydrocortisone	13341503	1
fargron	Hydrocortisone	13K22-B01-288284	1
Caelo	Hydrocortisone	13341508	4
Fagron	Hydrocortisone	14B04-B02-293423	3
Anzag	Hydrocortisone	1206018-01	1
Caelo	Hydrocortisone	13341511	3
Phönix Caesar u. Loretz	Hydrocortisone	13225507	1
Phönix	Hydrocortisone	13341508	1
Fagron	Hydrocortisone	K05B20131101	1
Caelo	Hydrocortisone	14115107	9
Fagron	Hydrocortisone	14B04-B02	2
Euro OTC	Hydrocortisone	1408023-01	4
Fagron	Hydrocortisone	13341510	1
Sanacorp	Hydrocortisone	13341509	1
Gehe	Hydrocortisone	1405001-01	1
Caelo	Hydrocortisone	14115108	2
Euro OTC	Hydrocortisone	1405001	1
Euro OTC	Hydrocortisone	1405001-01	2
Caelo	Hydrocortisone	14115105	3
Phönix	Hydrocortisone	1408023-01	1
Caelo	Hydrocortisone	14301305	4
Fagron	Hydrocortisone	13H08-B01-285473	1
Caelo	Hydrocortisone	13342504	1
Caelo	Hydrocortisone	14115103	2
Caelo	Hydrocortisone	14301306	4
Caelo	Hydrocortisone	14115104	1
Anzag	Hydrocortisone	14301306	1
Caelo	Hydrocortisone	14301312	5
Caelo	Hydrocortisone	14301310	13
Caelo	Hydrocortisone	140301305	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone	14301311	9
Fagron	Hydrocortisone	14B04-B02-293424	4
Gehe,27.0415	Hydrocortisone	14301310	1
Berkel AHK	Hydrocortisone	14301305	1
Fagron	Hydrocortisone	14B04-B02-293422	2
Euro OTC	Hydrocortisone	1501034-01	8
Caelo	Hydrocortisone	1501034-01	2
Caelo	Hydrocortisone	14b04-B02-293422	1
Caelo	Hydrocortisone	15021105	4
Caelo	Hydrocortisone	15021106	3
Caelo	Hydrocortisone	14301304	1
Caelo	Hydrocortisone	14301313	4
Caelo	Hydrocortisone	14301307	1
AHD;19.06.15;18,70EUR	Hydrocortisone	14301306	1
Caesar&loretz,Phoenix	Hydrocortisone	15021105	1
Caelo	Hydrocortisone	15021107	11
Fagron	Hydrocortisone	14/05-B02-300227	2
Caesar&loretz,Phoenix	Hydrocortisone	15181004	1
Anzag	Hydrocortisone	1501034-01	1
Phönix Gotha	Hydrocortisone	15181004	1
Caelo	Hydrocortisone	15181004	6
Caelo	Hydrocortisone	15021104	6
Nachprüfung 2312	Hydrocortisone	10282201	1
Fagron	Hydrocortisone	14105-B02-300228	1
Euro OTC	Hydrocortisone	1505016-01	28
Caelo	Hydrocortisone	15181006	16
Caelo	Hydrocortisone	15181003	7
Phönix Gotha	Hydrocortisone	15021107	1
Caelo	Hydrocortisone	15181014	6
Fagron	Hydrocortisone		1
Fagron	Hydrocortisone	13K22-B01-288282	1
Euro OTC	Hydrocortisone	150516-01	1
Caesar & Loretz GmbH	Hydrocortisone	15021107	1
Caelo	Hydrocortisone	15181007	5
Laborchemie Apolda/Phönix	Hydrocortisone	15181004	1
Bombastus	Hydrocortisone	14I05-B02-300227	1
Caelo	Hydrocortisone	15216101	6
Caelo	Hydrocortisone	15181013	9
Caelo	Hydrocortisone	15278702	6
Caelo	Hydrocortisone	15278703	7
Fagron	Hydrocortisone	14I05-B02	2
Caelo	Hydrocortisone	15181012	12
Fagron	Hydrocortisone	13H08-B01-285469	1
sanacorp	Hydrocortisone	15181013	1
Fagron	Hydrocortisone	15D14-B02-311696	5
Caelo	Hydrocortisone	1518013	1
Caelo	Hydrocortisone	15181008	1
Caelo	Hydrocortisone	15181012/20160309/10	1
Euro OTC	Hydrocortisone	150501601	1
Fagron	Hydrocortisone	14/05-B02-300227	1
phönix	Hydrocortisone	15181013	1
sanacorp	Hydrocortisone	15181012	1
Caelo	Hydrocortisone	260416v4	1
Caelo	Hydrocortisone	15278705	10
Euro OTC	Hydrocortisone	15278703	1
Caelo	Hydrocortisone	16004604	18
Caelo	Hydrocortisone	16004607	14
Euro OTC	Hydrocortisone	157015	2
Euro OTC	Hydrocortisone	1509029-01	24
Euro OTC	Hydrocortisone	150929-01	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Hydrocortisone	15181012	1
Caelo	Hydrocortisone	15278706	6
Euro OTC	Hydrocortisone	1505010601	1
Euro OTC	Hydrocortisone	1509029	1
Caelo	Hydrocortisone	16004605	10
Fagron	Hydrocortisone	15D14-B02	1
Gehe	Hydrocortisone	1509029-01	1
Fagron	Hydrocortisone	15/25-B01-313084	1
Fagron	Hydrocortisone	15I04-B03-315021	1
Bionorica	Hydrocortisone	16004604	1
Caesar&Loretz GmbH	Hydrocortisone	12104308	1
Caelo	Hydrocortisone	3081604	1
Sanacorp	Hydrocortisone	16004607	1
Phoenix	Hydrocortisone	1509029-01	1
Caelo	Hydrocortisone	16004603	9
Caelo	Hydrocortisone	16004608	7
Euro OTC	Hydrocortisone	150902	1
Fagron	Hydrocortisone	15/25-B01-318727	1
Fagron	Hydrocortisone	15125-B01-318486	1
AHL	Hydrocortisone	15125-B01-313084	1
Caelo	Hydrocortisone	130617H	1
Caelo	Hydrocortisone	16004611	7
Fagron	Hydrocortisone	14105-B02-300227	1
Caelo	Hydrocortisone	1518012	1
Caelo	Hydrocortisone	16095202	10
Caelo	Hydrocortisone	16095201	18
Anzag	Hydrocortisone	1509229-01	1
Euro OTC	Hydrocortisone	715Q-01719	1
Upjohn/Phönix	Hydrocortisone	1509029-01	1
Caesar & Loretz GmbH	Hydrocortisone	16004612	1
Fagron	Hydrocortisone	16H01-B01-324944	5
Fagron	Hydrocortisone	16A19-B06-321982	1
Caelo	Hydrocortisone	16095209	5
Caelo	Hydrocortisone	16095203	6
/ AHD	Hydrocortisone	16095202	1
Caelo	Hydrocortisone	16004612	6
Fagron	Hydrocortisone	1509029-01	1
Fagron	Hydrocortisone	16A19-B06-320970	20
Caelo	Hydrocortisone	16095210	15
Caelo	Hydrocortisone	1509029-01	2
Caelo	Hydrocortisone		2
Caelo	Hydrocortisone	16095207	7
Caelo	Hydrocortisone	16272305	6
Caelo	Hydrocortisone	16095212	5
Sanacorp	Hydrocortisone	1509029-01	1
Caelo	Hydrocortisone	16004612/2020317	1
Caelo	Hydrocortisone	16095213	6
Caelo	Hydrocortisone	1140317	1
Caelo	Hydrocortisone	16272306	5
Caesar&Loretz GmbH,Anza...	Hydrocortisone	16272305	1
Euro OTC	Hydrocortisone	150902901	1
Caelo	Hydrocortisone	16272304	7
Gehe	Hydrocortisone	16272306	1
Allianz Healthcare	Hydrocortisone	1509029-01	1
Noweda	Hydrocortisone	16004612	1
Fagron	Hydrocortisone	16H01-B01-326071	2
Phoenix	Hydrocortisone	16095207	1
Euro OTC	Hydrocortisone	1611016-01	26
Caelo	Hydrocortisone	16255606	1
Kehr	Hydrocortisone	16095213	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone	1672305	1
Caelo	Hydrocortisone	16255607	3
Fagron	Hydrocortisone	16j26-b04-330339	1
Caelo	Hydrocortisone	16272311	2
Caelo	Hydrocortisone	1611016-01	1
Euro/ Phönix	Hydrocortisone	1509029-01	1
Caelo	Hydrocortisone	16095213-20170704Ma7	1
Caelo	Hydrocortisone	16255603	4
Caelo	Hydrocortisone	16255604	1
Fagron	Hydrocortisone	16A19-B06	1
GEHE	Hydrocortisone	16272311	1
Caelo	Hydrocortisone	16272308	4
Caelo	Hydrocortisone	16255680	1
Caelo	Hydrocortisone	17090003	3
Caelo	Hydrocortisone	16255608	9
Delta	Hydrocortisone	16H01-B01-326071	1
Caelo	Hydrocortisone	17119402	6
Fagron	Hydrocortisone	16H01-B01	1
Fagron	Hydrocortisone	16J26-B04-330340	1
Noweda	Hydrocortisone	16255608	1
Caelo	Hydrocortisone	17119404	1
Finteler Apotheke	Hydrocortisone	1611016-01	1
Fagron	Hydrocortisone	17E10-B04-334857	2
Euro OTC	Hydrocortisone	3817A-01719	1
Caelo	Hydrocortisone	170921HA/17090003	1
Caelo	Hydrocortisone	17119407	16
Kehr	Hydrocortisone	17119407	1
Caelo	Hydrocortisone	17119405	13
Fragon/Sanacorp	Hydrocortisone	17E10-B04-335056	1
gehe	Hydrocortisone	16255607	1
Gehe	Hydrocortisone	17E10-B04-335656	1
Caecelo	Hydrocortisone	17090005	1
Fagron	Hydrocortisone	17C13-B06-333045	2
Fagron	Hydrocortisone	17E10-B04	1
Caelo	Hydrocortisone	1672308	1
Fagron	Hydrocortisone	16272311	1
Caelo	Hydrocortisone	1719402-20171106Ma2	1
Caelo	Hydrocortisone	17119406	4
Caelo	Hydrocortisone	17090005	5
Euro OTC	Hydrocortisone	161016-01	1
Caecelo/Krieger	Hydrocortisone	17119406	1
Caelo	Hydrocortisone	17119403	10
Fagron	Hydrocortisone	17E10-B04-334858	3
Caelo	Hydrocortisone	17119410	4
Caelo	Hydrocortisone	17256602	18
Euro OT/Anzag	Hydrocortisone	1611016-01	3
Caesar & Loretz	Hydrocortisone	17256603	2
Fagron	Hydrocortisone	17E10-B04-336436	2
Fagron	Hydrocortisone	17E10-B04-336435	1
Caelo	Hydrocortisone	17256804	1
Caelo	Hydrocortisone	17229410	1
Caelo	Hydrocortisone	17119405	1
Caelo	Hydrocortisone	17256605	8
Caelo	Hydrocortisone	17256604	12
Noweda	Hydrocortisone	1611016-01	1
Phönix	Hydrocortisone	1611016-01	2
Caelo	Hydrocortisone	17256603	3
Caelo	Hydrocortisone	17256607	2
Euro OTC	Hydrocortisone	17351202	1
Kehr	Hydrocortisone	17256602	1

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Supplier	Substance	Batch	Spectra
Gehe	Hydrocortisone	17256604	1
Caelo	Hydrocortisone	17351202	6
Sanacorp	Hydrocortisone	17256604	1
Caelo	Hydrocortisone	17351205	18
Euro OTC	Hydrocortisone	17256603	1
Fiebig	Hydrocortisone	17256602	1
Fagron	Hydrocortisone	17G25-B02-340864	1
Caelo	Hydrocortisone	17526602	1
Fagron	Hydrocortisone	17E10B04335656	1
Fagron	Hydrocortisone	17351205	1
Caelo	Hydrocortisone	16255608NP	1
Caelo	Hydrocortisone	3110456	1
Caelo	Hydrocortisone	K05B20160909	1
Caelo	Hydrocortisone	17351203	7
Fagron	Hydrocortisone	17/12-B05-344220	1
Caelo	Hydrocortisone	17351209	3
Fagron	Hydrocortisone	17-12B05-342611	1
Caelo	Hydrocortisone	17351206	6
Caelo	Hydrocortisone	18091501	4
Fagron	Hydrocortisone	17I12-B05-34554	1
Caelo	Hydrocortisone	1726603	1
Euro OTC	Hydrocortisone	210818A	1
Caelo	Hydrocortisone	17351209-20180830Ma3	1
Caelo/ Noweda	Hydrocortisone	17351209	1
Fagron	Hydrocortisone	18091501	1
Caelo	Hydrocortisone	18091503	4
Euro OTC	Hydrocortisone	1802009-01	4
Caelo	Hydrocortisone	18091507	3
Fagron	Hydrocortisone	K05M20170702	1
Caelo	Hydrocortisone	18091501-H20181115Ma	3
Caelo	Hydrocortisone	18091505	4
Caelo	Hydrocortisone	18091502	1
Caelo	Hydrocortisone	18091508	1
Caelo	Hydrocortisone	18091519	1
Caelo	Hydrocortisone	18091506	1

- 77 733 spectra from 564 *Apo-Ident* customers from a total of 25 880 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	386	0	74 110
Type B	0	751	3	126 138
Type C	0	1092	104	77 733

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.4456 %)
Type B	100.0000 % (> 99.9901 %)	99.6021 % (> 99.2042 %)
Type C	100.0000 % (> 99.8817 %)	91.3043 % (> 91.0535 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22838	22838	0.00	44.56
21293	21899	4.96	51.99
22829	22838	6.63	40.93
21461	22910	6.12	51.15
21899	21899	0.00	53.27
22910	22910	0.00	52.99
22928	22910	2.00	53.43

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Hydrocortisone acetate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20010-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hydrocortisone acetate; Hydrocortisoni acetat

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Hydrocortisone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Hydrocortisone a...	1209003-01	21295	40	20121108
Euro OTC	Hydrocortisone a...	1508029	21889	40	20150902*
Fagron	Hydrocortisone a...	15A30-B09-307090	22241	40	20150226
Euro OTC	Hydrocortisone a...	1604052	22564	40	20160525*
Euro OTC	Hydrocortisone a...	1209003-01	21295SI	30	20121108
Euro OTC	Hydrocortisone a...	1508029	21889SI	29	20150902*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 219 spectra of 6 reference samples from the substance/substance group *Hydrocortisone acetate*. These samples are listed above in the [calibration samples](#) section.
- 74277 spectra from a total of 1619 batches from further 372 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 [†].

- 508 spectra of 17 reference samples from the substance/substance group *Hydrocortisone acetate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrocortisone acetate	13291708	21462	60
Euro OTC	Hydrocortisone acetate	1508029	21889 [†]	20
Fagron	Hydrocortisone acetate	15A30-B09-307090	22241 [†]	20
Caelo	Hydrocortisone acetate	16238706	23115	40
Caelo	Hydrocortisone acetate	170862	23328	40
Euro OTC	Hydrocortisone acetate	1706021	23559	40
Euro OTC	Hydrocortisone acetate	1805010	24130	40
Caelo	Hydrocortisone acetate	182780	24392	40
Euro OTC	Hydrocortisone acetate	1209003-01	21295SI [†]	15
Euro OTC	Hydrocortisone acetate	1508029	21889SI [†]	15
Fagron	Hydrocortisone acetate	15A30-B09-307090	22241SI	24
Euro OTC	Hydrocortisone acetate	1604052	22564SI	30
Caelo	Hydrocortisone acetate	16238706	23115SI	20
Caelo	Hydrocortisone acetate	170862	23328SI	21
Euro OTC	Hydrocortisone acetate	1706021	23559SI	30
Euro OTC	Hydrocortisone acetate	1805010	24130SI	21
Caelo	Hydrocortisone acetate	182780	24392SI	32

*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*.

- 126384 spectra from a total of 2779 batches from further 781 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.

- 1504 spectra from 412 *Apo-Ident* customers from 273 batches from the substance/substance group *Hydrocortisone acetate*.

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	1406211718	1
Caelo	Hydrocortisone acetate	15061207	1
Caelo	Hydrocortisone acetate	12008405	4
Caelo	Hydrocortisone acetate	11263905	1
Caelo	Hydrocortisone acetate	11098604	1
Caelo	Hydrocortisone acetate	11098615	1
Caelo	Hydrocortisone acetate	11263913	1
Caelo	Hydrocortisone acetate	11263916	1
Caelo	Hydrocortisone acetate	11263915	2
Caelo	Hydrocortisone acetate	11263917	3
Euro OTC	Hydrocortisone acetate	1107004-03	2
Euro OTC	Hydrocortisone acetate	1112031-01	11
Caelo	Hydrocortisone acetate	12008402	2
EuRho	Hydrocortisone acetate	1107004-03	1
Caelo	Hydrocortisone acetate	12182403	5
Caelo	Hydrocortisone acetate	10301904	1
Phönix	Hydrocortisone acetate	12A13-N02	1
Euro OTC	Hydrocortisone acetate	911I-01718	1
Caelo	Hydrocortisone acetate	12183403	1
Fagron	Hydrocortisone acetate	12K15-N04	6
Caelo	Hydrocortisone acetate	12182404	19
Noweda	Hydrocortisone acetate	1112031-02	1
Caelo	Hydrocortisone acetate	12182402	10
Sanacorp	Hydrocortisone acetate	1107004-03	1
Phoenix	Hydrocortisone acetate	12182402	1
Anzag	Hydrocortisone acetate	1112031-02	1
Caelo	Hydrocortisone acetate	18011304	1
Sanacorp	Hydrocortisone acetate	11263913	1
Sanacorp	Hydrocortisone acetate	12182404	2
Bombastus	Hydrocortisone acetate	2712M01718	1
Caelo	Hydrocortisone acetate	12182405	17
Caesar&loretz,Phoenix	Hydrocortisone acetate	12182405	1
Caelo	Hydrocortisone acetate	3110491	1
Caelo	Hydrocortisone acetate	2612M01718	1
Caelo	Hydrocortisone acetate	11263902	1
Euro OTC	Hydrocortisone acetate	1112031-02	3
Caesar & Loretz GmbH	Hydrocortisone acetate	12182405	1
Fagron	Hydrocortisone acetate	11/01-N05	1
Caelo	Hydrocortisone acetate	1213M-01718	1
Fagron	Hydrocortisone acetate	1112031	1
Caelo	Hydrocortisone acetate	12330106	4
Caelo	Hydrocortisone acetate	11098612	1
Caelo	Hydrocortisone acetate	12330103	8
Caelo	Hydrocortisone acetate	1205034-01	3
Phönix	Hydrocortisone acetate	1112031-01	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	12330102	7
Caelo	Hydrocortisone acetate	7051303	1
Caelo	Hydrocortisone acetate	12182408	2
Caelo	Hydrocortisone acetate	12330107	8
Caelo	Hydrocortisone acetate		6
Noweda/ Pharmacia & Upj...	Hydrocortisone acetate	1205034-01	1
Euro OTC	Hydrocortisone acetate	1205034-01	22
Fagron	Hydrocortisone acetate	12330107	1
Phönix Gotha	Hydrocortisone acetate	12182405	1
Caelo	Hydrocortisone acetate	12330110	2
Fagron	Hydrocortisone acetate	13A03-N04	4
Euro OTC	Hydrocortisone acetate	HCAZ11004K	1
Caelo	Hydrocortisone acetate	12330104	9
Caelo	Hydrocortisone acetate	12330105	2
Sanacorp	Hydrocortisone acetate	12330103	1
Caelo	Hydrocortisone acetate	1112031-02	1
Phoenix	Hydrocortisone acetate	12330107	1
Nachprüfung	Hydrocortisone acetate		1
Fagron	Hydrocortisone acetate	13B25-N04	2
Caelo	Hydrocortisone acetate	12330112	13
Caelo	Hydrocortisone acetate	12330108	14
Fagron	Hydrocortisone acetate	3613A-01718	1
AHD	Hydrocortisone acetate	1205034-01	1
Phönix	Hydrocortisone acetate	12K15-No4	1
Caelo	Hydrocortisone acetate	12330111	3
Caelo	Hydrocortisone acetate	12330116	10
Caelo	Hydrocortisone acetate	27091307	1
Caelo	Hydrocortisone acetate	12330114	1
Klenk	Hydrocortisone acetate	1112031-01	1
Phönix	Hydrocortisone acetate	AKD8	1
Phönix	Hydrocortisone acetate	1205034-01	1
Caelo	Hydrocortisone acetate	13155302	7
Sanacorp	Hydrocortisone acetate	13155302	2
Fagron	Hydrocortisone acetate	13E31-No2	1
Fagron	Hydrocortisone acetate	13E31-N02	2
Euro OTC	Hydrocortisone acetate	120503401	3
Caelo	Hydrocortisone acetate	13155304	5
Fagron	Hydrocortisone acetate	8563642	1
Caelo	Hydrocortisone acetate	13155308	8
Caelo	Hydrocortisone acetate	13155303	7
Caelo	Hydrocortisone acetate	131553080	1
Fagron	Hydrocortisone acetate	13155311	1
Fagron	Hydrocortisone acetate	13G09-N08	4
Caelo	Hydrocortisone acetate	25101201	1
Euro OTC	Hydrocortisone acetate	1209003-01	20
Caelo	Hydrocortisone acetate	12330113	1
Caelo	Hydrocortisone acetate	12330111-3507411061	1
Caeolo/Noweda	Hydrocortisone acetate	13155303	1
Caelo	Hydrocortisone acetate	13155307	2
Caelo	Hydrocortisone acetate	13291706	9
Euro OTC	Hydrocortisone acetate	120900301	2
Caelo	Hydrocortisone acetate	13291709	4
Caelo	Hydrocortisone acetate	13G09-N08	2
Phönix	Hydrocortisone acetate	1112031-02	1
Caelo	Hydrocortisone acetate	13291707	12
AHD	Hydrocortisone acetate	13291707	1
Caelo	Hydrocortisone acetate	1209003-01	6
Caelo	Hydrocortisone acetate	13291708	5
Caelo	Hydrocortisone acetate	13155306	4
Cealo / Noweda	Hydrocortisone acetate	13291707	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	1391704	1
Caelo	Hydrocortisone acetate	13291704	2
Caelo	Hydrocortisone acetate	3110516	1
Caelo	Hydrocortisone acetate	13291705	4
Caelo	Hydrocortisone acetate	1391706	1
Caelo	Hydrocortisone acetate	14043903	11
Noweda	Hydrocortisone acetate	13G09-N08	1
Caelo	Hydrocortisone acetate	14043907	13
Euro OTC	Hydrocortisone acetate	12090003-01	3
Fagron	Hydrocortisone acetate	14043903	1
Sanacorp	Hydrocortisone acetate	13291704	1
Caelo	Hydrocortisone acetate	1403903	1
Euro OTC	Hydrocortisone acetate	1404017-01	11
Sanacorp	Hydrocortisone acetate	14043903	1
GEHE 03.07.2014	Hydrocortisone acetate	14043903	1
Caelo	Hydrocortisone acetate	13291701	1
Phönix	Hydrocortisone acetate	12182405	1
Anzag	Hydrocortisone acetate	1209003-01	1
Pharmacia&Upjohn Comp. ...	Hydrocortisone acetate	1209003-01	1
Caelo	Hydrocortisone acetate	14043904	10
Caelo	Hydrocortisone acetate	13291711	7
Euro/Gehe	Hydrocortisone acetate	1404017-01	1
Fagron	Hydrocortisone acetate	13J31B07290061	1
Hedinger/Gehe	Hydrocortisone acetate	1112031-02	1
Caelo	Hydrocortisone acetate	14043901	10
Caelo	Hydrocortisone acetate	14043902	8
Fagron	Hydrocortisone acetate	13J31-B07	3
Fagron	Hydrocortisone acetate	14043906	1
Caelo	Hydrocortisone acetate	14043906	6
Phoenix	Hydrocortisone acetate	1568/05131813	1
Caelo	Hydrocortisone acetate	14144806	11
Phoenix	Hydrocortisone acetate	1209003-01	1
Caelo	Hydrocortisone acetate	14043905	7
Gehe	Hydrocortisone acetate	14043905	1
Fagron	Hydrocortisone acetate	13J31-B07-290061	2
Caelo	Hydrocortisone acetate	14144805	17
Euro OTC	Hydrocortisone acetate	1404017-02	5
Fagron	Hydrocortisone acetate	HC0024	1
Apomix/Noweda	Hydrocortisone acetate	1404017-02	1
Phönix	Hydrocortisone acetate	14144804	1
Euro OTC	Hydrocortisone acetate	1409005-01	13
Sanacorp	Hydrocortisone acetate	1409005-01	3
Phoenix 14.01.2015 EK: ...	Hydrocortisone acetate	14043902	1
Fagron	Hydrocortisone acetate	14043905	1
Caelo	Hydrocortisone acetate	14144803	7
Caelo	Hydrocortisone acetate	14144807	5
Euro/ Sanacorp	Hydrocortisone acetate	1409005-01	1
Euro OTC	Hydrocortisone acetate	140900501	1
Fagron	Hydrocortisone acetate	14A13-B04-294158	2
Lihua/phönix	Hydrocortisone acetate	K06A20140801M	1
Euro OTC	Hydrocortisone acetate	1409005-02	4
Fagron	Hydrocortisone acetate	14A13-B04	1
Caelo	Hydrocortisone acetate	14301405	23
Caelo	Hydrocortisone acetate	14301402	6
AHD;05,02,15; 12.48EUR	Hydrocortisone acetate	14144805	1
Euro OTC	Hydrocortisone acetate	1501035-01	11
Caelo	Hydrocortisone acetate	14144802	1
Euro OTC	Hydrocortisone acetate	150103501	3
EuRho/Phoenix	Hydrocortisone acetate	1209003-01	1
	Hydrocortisone acetate	14043902	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Hydrocortisone acetate	1404017-03	1
Caelo	Hydrocortisone acetate	14144804	3
Caelo	Hydrocortisone acetate	14301406	16
Phoenix Goettin	Hydrocortisone acetate	1209003-01	1
Caelo	Hydrocortisone acetate	1501035	1
Fagron	Hydrocortisone acetate	13F25-B05-300290	2
Caelo	Hydrocortisone acetate	14301401	8
Fagron	Hydrocortisone acetate	14144804	1
Fagron	Hydrocortisone acetate	14301402	1
Sanacorp	Hydrocortisone acetate	1501035-01	1
Gehe	Hydrocortisone acetate	1501035-01	1
Caesar&Loretz GmbH/Anzag	Hydrocortisone acetate	14301405	2
Caelo	Hydrocortisone acetate	14301407	12
Euro OTC	Hydrocortisone acetate	1505008-01	43
Caelo	Hydrocortisone acetate	14301404	6
Fagron	Hydrocortisone acetate	13/31-B07-290061	1
Caelo	Hydrocortisone acetate	14301408	5
Noweda 17.07.2015	Hydrocortisone acetate	14301403	1
Caelo	Hydrocortisone acetate	15A07-B03-306545	1
Euro OTC	Hydrocortisone acetate	140900502	1
Euro OTC	Hydrocortisone acetate	1502000801	1
Fagron	Hydrocortisone acetate	13J31-B07-290062	2
Fagron	Hydrocortisone acetate	15A03-B09-307133	1
caesar	Hydrocortisone acetate	14301402	1
Caelo	Hydrocortisone acetate	15067004	17
Caelo	Hydrocortisone acetate	15067003	11
Caelo	Hydrocortisone acetate	14301403	4
Caelo	Hydrocortisone acetate	15067005	18
Caelo/Anzag	Hydrocortisone acetate	15067003	1
Fagron	Hydrocortisone acetate	15A07-B03-306545	1
Euro OTC	Hydrocortisone acetate	1508029-01	27
Fagron	Hydrocortisone acetate	15A30-B09-307133	4
Caelo	Hydrocortisone acetate	15067010	2
Bombastus	Hydrocortisone acetate	123Validierung	1
Caesar & Loretz GmbH	Hydrocortisone acetate	15067004	1
Euro OTC	Hydrocortisone acetate	L68934	1
Caelo	Hydrocortisone acetate	301115	1
Caelo	Hydrocortisone acetate	15067011	6
Euro OTC	Hydrocortisone acetate	150500801	3
Caelo	Hydrocortisone acetate	15067006	7
Euro OTC	Hydrocortisone acetate	1505008	1
Fagron	Hydrocortisone acetate	15A03-B09-307300	1
Klenk	Hydrocortisone acetate	14301401	1
sanacorp	Hydrocortisone acetate	14301406	1
Gatt-Koller	Hydrocortisone acetate	1734/05154415	1
Europh-Gehe	Hydrocortisone acetate	1508029-01	1
Caelo	Hydrocortisone acetate	15216204	2
Caelo	Hydrocortisone acetate	15356902	13
Caelo	Hydrocortisone acetate	15356904	8
Fagron	Hydrocortisone acetate	15H24-B01-314236	1
Caelo	Hydrocortisone acetate	1505008-01	2
Caelo	Hydrocortisone acetate	15356901	13
Caelo	Hydrocortisone acetate	15356903	15
Fagron	Hydrocortisone acetate	15067006	1
Euro OTC	Hydrocortisone acetate	14301406	1
Fagron	Hydrocortisone acetate	15H24-B01-316480	1
Caelo	Hydrocortisone acetate	16004402	10
Caelo	Hydrocortisone acetate	15067013	7
Phoenix	Hydrocortisone acetate	15A30-B09	1
Caesar&Loretz GmbH/AHD	Hydrocortisone acetate	15356903	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	1430140	1
Fagron	Hydrocortisone acetate	M39171	1
Caelo	Hydrocortisone acetate	15H24-B01-314236	2
Fagro/Gehe	Hydrocortisone acetate	15A07-B03306545	1
Fagron	Hydrocortisone acetate	15H24-B01	1
phönix	Hydrocortisone acetate	15356901	2
Caelo	Hydrocortisone acetate	16004403	8
Caelo	Hydrocortisone acetate	1536902	1
Fagron	Hydrocortisone acetate	15J28-B12-317771	1
Caelo	Hydrocortisone acetate	16004407	15
Caelo	Hydrocortisone acetate	16004405	7
Caelo	Hydrocortisone acetate	20160727Ma2	1
Phoenix	Hydrocortisone acetate	16004403	1
Euro OTC	Hydrocortisone acetate	1604052-01	49
Euro OTC	Hydrocortisone acetate	508029-01	2
Euro OTC	Hydrocortisone acetate	1508029	2
Caelo	Hydrocortisone acetate	16004406	12
Phoenix	Hydrocortisone acetate	15J28-B12	1
Euro/Alliance Healthcare	Hydrocortisone acetate	1508029-01	1
Caolo- Noweda	Hydrocortisone acetate	15067006	1
Caol/Phoenix	Hydrocortisone acetate	16004402	1
Caelo	Hydrocortisone acetate	16004408	12
Fagron	Hydrocortisone acetate	15h24-b01-314236	1
Caelo	Hydrocortisone acetate	1600406	1
Caelo	Hydrocortisone acetate	160629HA	1
Euro OTC	Hydrocortisone acetate	16004406	1
Fagron	Hydrocortisone acetate	15J28-B12	1
Caesar u Loretz	Hydrocortisone acetate	15067003	1
Bombastus	Hydrocortisone acetate	15356903	1
Caelo	Hydrocortisone acetate	160044402	1
Caesar & Loretz GmbH	Hydrocortisone acetate	16004402	1
Caelo	Hydrocortisone acetate	16095404	21
Fagron	Hydrocortisone acetate	NCEHAC151101	1
Caelo	Hydrocortisone acetate	16095406	14
Caesar & Loretz	Hydrocortisone acetate	16095404	1
Caesar & Loretz GmbH	Hydrocortisone acetate	16095406	2
Caelo	Hydrocortisone acetate	15H24B01-316480	1
Caelo	Hydrocortisone acetate	16004404	1
GEHE	Hydrocortisone acetate	1604052-01	1
Caelo	Hydrocortisone acetate	16095407	17
Caelo	Hydrocortisone acetate	1604052-01	4
Fagron	Hydrocortisone acetate	16C15-B04-321459	1
Caelo	Hydrocortisone acetate	16095408	3
Euro OTC	Hydrocortisone acetate	160405201	2
Caelo	Hydrocortisone acetate	16095405	12
Caelo	Hydrocortisone acetate	160044003	1
Caelo	Hydrocortisone acetate	16C15-B04-321459	1
Caelo	Hydrocortisone acetate	1508029-01	1
SanacorpWE:13.02.2017 ...	Hydrocortisone acetate	1604052-01	1
Caelo	Hydrocortisone acetate	16238704	5
Caelo	Hydrocortisone acetate	16238708	16
Caesar & Loretz GmbH	Hydrocortisone acetate	16095405	1
AHD 07.03.2017 EK: 5,33	Hydrocortisone acetate	16004407	1
Gehe	Hydrocortisone acetate	16004408	1
Caelo	Hydrocortisone acetate	16238706	17
Caelo	Hydrocortisone acetate	166004407	1
Euro OTC	Hydrocortisone acetate	150802901	1
phönix	Hydrocortisone acetate	16238708	1
Caelo	Hydrocortisone acetate	16238710	6
Caesar&Loretz GmbH,Phön...	Hydrocortisone acetate	16238708	1

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Supplier	Substance	Batch	Spectra
Gehe	Hydrocortisone acetate	16238710	1
Sanacorp	Hydrocortisone acetate	16238706	1
Noweda/Euro	Hydrocortisone acetate	1501035-01	1
Noweda/Apomix	Hydrocortisone acetate	16095407	1
Fagron	Hydrocortisone acetate	1604052-01	1
Caesar & Loretz GmbH	Hydrocortisone acetate	16004408	1
Fagron	Hydrocortisone acetate	16H18-B04-325093	2
Anzag	Hydrocortisone acetate	16238708	1
Finteler Apotheke	Hydrocortisone acetate	1604052-01	2
Noweda	Hydrocortisone acetate	16095407	1
Caelo	Hydrocortisone acetate	16238714	8
Caelo	Hydrocortisone acetate	16238712	19
Caelo	Hydrocortisone acetate	16238707	8
Alliance	Hydrocortisone acetate	1604052-01	1
Fagron	Hydrocortisone acetate	160405201	1
phönix	Hydrocortisone acetate	16238712	1
Caelo	Hydrocortisone acetate	1604052	1
Caelo	Hydrocortisone acetate	16238709	6
Fagron	Hydrocortisone acetate	16J28-B05-330083	1
Anzag	Hydrocortisone acetate	16238712	1
Fagron	Hydrocortisone acetate	16H18-B04-327325	1
Sanacorp	Hydrocortisone acetate	16238710	1
Caelo	Hydrocortisone acetate	17086203	7
GEHE	Hydrocortisone acetate	16238712	1
Caelo	Hydrocortisone acetate	16238713	5
Caelo	Hydrocortisone acetate	16238705	1
Caelo	Hydrocortisone acetate	17086205	4
Caelo	Hydrocortisone acetate	170804HA/1604052-01	1
Anzag	Hydrocortisone acetate	16238713	1
Fagron	Hydrocortisone acetate	16J28-B05	1
Caelo	Hydrocortisone acetate	17086205-20170818Ma3	1
Caelo	Hydrocortisone acetate	16238713-20170818Ma2	1
Sanacorp	Hydrocortisone acetate	16238708	1
Euro OTC	Hydrocortisone acetate	2604052-01	1
Euro OTC	Hydrocortisone acetate	170830HA/1706021-01	1
Euro OTC	Hydrocortisone acetate	1508029-02	1
Caelo	Hydrocortisone acetate	17086206	6
Anzag	Hydrocortisone acetate	17086206	2
Caelo	Hydrocortisone acetate	17086204	10
Fagron	Hydrocortisone acetate	17086211	3
Fagron	Hydrocortisone acetate	7C10-B01-333961	1
Fagron	Hydrocortisone acetate	17C10-B01-333962	3
Caelo	Hydrocortisone acetate	17086204	1
Caelo	Hydrocortisone acetate	17086212	1
Caelo	Hydrocortisone acetate	17086207	3
Euro OTC	Hydrocortisone acetate	17086203	1
Caelo	Hydrocortisone acetate	163163055402	1
Euro OTC	Hydrocortisone acetate	1706021-01	19
Caelo	Hydrocortisone acetate	17219706	12
Caelo	Hydrocortisone acetate	171106HA/17086204	1
Caelo	Hydrocortisone acetate	1706021-01	3
Caelo	Hydrocortisone acetate	17219704	11
GEHE	Hydrocortisone acetate	16238713	1
GEHE	Hydrocortisone acetate	1706021-01	2
Caelo	Hydrocortisone acetate	16095410	2
Caelo	Hydrocortisone acetate	170856206	1
	Hydrocortisone acetate	333961	1
Fagron	Hydrocortisone acetate	17G03-B06-338750	1
Caesar & Loretz/AHD	Hydrocortisone acetate	17219706	1
Euro OT/Anzag	Hydrocortisone acetate	1706021-01	2

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Supplier	Substance	Batch	Spectra
Cealo/Gehe	Hydrocortisone acetate	16095410	2
Caelo	Hydrocortisone acetate	170602101	1
Fagron	Hydrocortisone acetate	17C10	2
Fagron	Hydrocortisone acetate	17C10-B01-335774	1
Caelo	Hydrocortisone acetate	17086211	1
Caelo	Hydrocortisone acetate	17219705	13
Hedinger/Sanacorp	Hydrocortisone acetate	1706021-01	2
gehe	Hydrocortisone acetate	17219707	1
Caelo	Hydrocortisone acetate	17219702	9
Caelo	Hydrocortisone acetate	17219708	11
EuRro/Anzag	Hydrocortisone acetate	1706021-01	2
Fiebig	Hydrocortisone acetate	1605410	1
Caelo	Hydrocortisone acetate	17219709	1
Caelo	Hydrocortisone acetate	17219707	15
Anzag	Hydrocortisone acetate	17219702	2
Caelo	Hydrocortisone acetate	180219HA/17219707	1
Fagron	Hydrocortisone acetate	17G03-B06-341843	1
Sanacorp	Hydrocortisone acetate	17219704	1
Noweda	Hydrocortisone acetate	17219706	1
Caelo	Hydrocortisone acetate	1605410	1
Caelo	Hydrocortisone acetate	172197085556	1
Kehr	Hydrocortisone acetate	1706021-01	2
Caelo	Hydrocortisone acetate	17219703	6
Euro OTC	Hydrocortisone acetate	170602-01	1
Anzag	Hydrocortisone acetate	17219703	1
Caelo	Hydrocortisone acetate	17219713	1
Allianz	Hydrocortisone acetate	17219705	1
EuRho	Hydrocortisone acetate	1706021-01	1
Caelo	Hydrocortisone acetate	17358403	4
GEHE	Hydrocortisone acetate	17219703	1
Euro OTC	Hydrocortisone acetate	17219709	1
Caelo	Hydrocortisone acetate	18142803	7
Caelo	Hydrocortisone acetate	17219714	1
Fagron	Hydrocortisone acetate	17G03-B06-345375	3
Euro OTC	Hydrocortisone acetate	1706021	1
Euro OTC	Hydrocortisone acetate	17219705	1
Caelo	Hydrocortisone acetate	172197055662	1
Caelo	Hydrocortisone acetate	18142805	5
Caelo	Hydrocortisone acetate	18142808	4
Fagron	Hydrocortisone acetate	17L19	2
Caelo	Hydrocortisone acetate	18142810	1
Gehe	Hydrocortisone acetate	17219705	1
Caelo	Hydrocortisone acetate	18142811	2
Caelo	Hydrocortisone acetate	18142802	3
Hepart	Hydrocortisone acetate	14144804	1
Fagron	Hydrocortisone acetate	17L19B04345374	1
Klenk	Hydrocortisone acetate	18142803	1
Caelo	Hydrocortisone acetate	18142806	7
Fagron	Hydrocortisone acetate	18142806	1
Fagron	Hydrocortisone acetate	17L19-B04-350448	1
Euro OTC	Hydrocortisone acetate	18142805	1
Euro OTC	Hydrocortisone acetate	1805010-01	3
Fagron	Hydrocortisone acetate	17L19-B04-348983	1
Caelo	Hydrocortisone acetate	18142805-H20181115Ma	1
Caelo	Hydrocortisone acetate	18142804	4
Euro OTC	Hydrocortisone acetate	17066021-01	1
Gehe	Hydrocortisone acetate	18142812	1
Fagro/Noweda	Hydrocortisone acetate	18142804	1
Caelo	Hydrocortisone acetate	18142807	2
Caesar & Loretz	Hydrocortisone acetate	18142815	2

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Supplier	Substance	Batch	Spectra
xxx	Hydrocortisone acetate		1
Sanacorp	Hydrocortisone acetate	18278006	1
Caelo	Hydrocortisone acetate	18278006	1

- 77 425 spectra from 565 *Apo-Ident* customers from a total of 25 871 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Hydrocortisone 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 *Hydrocortisone 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	219	0	74 277
Type B	0	505	3	126 384
Type C	0	1372	132	77 425

The substance/substance group *Hydrocortisone 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 % (> 99.9887 %)	100.0000 % (> 97.2603 %)
Type B	100.0000 % (> 99.9901 %)	99.4094 % (> 98.8189 %)
Type C	100.0000 % (> 99.8817 %)	91.2234 % (> 91.0239 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
22564	22564	0.00	43.40

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21295	21889	4.52	43.37
21889	21889	0.00	42.66
22241	21889	3.44	44.14

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Hydrocortisone butyrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21531-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hydrocortisone butyrate; Hydrocortisoni butyras micronisatum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Hydrocortisone butyrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Hydrocortisone b...	13I26-N01	21531	40	AR-15-FG-000944-01
Fagron	Hydrocortisone b...	14D23-B01-296716	21723	30	20140509
Fagron	Hydrocortisone b...	13I26-N01	21797	40	20130920
Fagron	Hydrocortisone b...	16F20-B05-323903	23182	40	20160805
Fagron	Hydrocortisone b...	13I26-N01	21797SI	30	20130920

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 5 reference samples from the substance/substance group *Hydrocortisone butyrate*. These samples are listed above in the [calibration samples](#) section.
- 74316 spectra from a total of 1620 batches from further 372 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 [†].

- 433 spectra of 14 reference samples from the substance/substance group *Hydrocortisone butyrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Hydrocortisone butyrate	13I26-N01	21531 [†]	20
Fagron	Hydrocortisone butyrate	14D23-B01-296716	21723 [†]	30
Fagron	Hydrocortisone butyrate	13I26-N01	21797 [†]	20
Fagron	Hydrocortisone butyrate	15J12-B03-322394	23721	40
Fagron	Hydrocortisone butyrate	15J12-B03-322394	23722	40
Fagron	Hydrocortisone butyrate	16J21-B01-333229	23743	40
Fagron	Hydrocortisone butyrate	16J21-B01-333229	23765	40
Fagron	Hydrocortisone butyrate	14D23-B01-296716	21723SI	48
Fagron	Hydrocortisone butyrate	13I26-N01	21797SI [†]	15
Fagron	Hydrocortisone butyrate	16F20-B05-323903	23182SI	20
Fagron	Hydrocortisone butyrate	15J12-B03-322394	23721SI	25
Fagron	Hydrocortisone butyrate	15J12-B03-322394	23722SI	22
Fagron	Hydrocortisone butyrate	16J21-B01-333229	23743SI	37
Fagron	Hydrocortisone butyrate	16J21-B01-333229	23765SI	36

- 126459 spectra from a total of 2784 batches from further 781 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](#).

[†]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.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Hydrocortisone butyrate*.

Supplier	Substance	Batch	Spectra
Fagron	Hydrocortisone butyrate	15G08-B16-314883	1

- 78 928 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	180	0	74 316
Type B	0	433	0	126 459
Type C	0	1	0	78 928

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.6143 %)
Type C	100.0000 % (> 99.8830 %)	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
23182	21531	8.06	32.75
21797	21531	2.40	24.99
21531	21531	0.00	20.32
21723	21531	11.23	30.20

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Hydroquinone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20091-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hydroquinone; Hydrochinonum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Hydroquinone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydroquinone	12288505	20884	40	20121015
Caelo	Hydroquinone	14026904	21468	40	20140122
Caelo	Hydroquinone	14281501	21791	40	AR-15-FG-008058-01
Caelo	Hydroquinone	14280110	21923	40	20141017
Caelo	Hydroquinone	15057004	21975	40	20150306
Caelo	Hydroquinone	15057001	22324	40	20150306
Caelo	Hydroquinone	15057001	22351	40	20150306

Validation samples

A total of 280 317 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 *Hydroquinone*. These samples are listed above in the [calibration samples](#) section.
- 74 216 spectra from a total of 1617 batches from further 372 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 8 reference samples from the substance/substance group *Hydroquinone*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydroquinone	14026904	21468 [†]	20
Caelo	Hydroquinone	14281501	21791 [†]	20
Caelo	Hydroquinone	14280110	21923 [†]	20
Caelo	Hydroquinone	15057004	21975 [†]	20
Caelo	Hydroquinone	15057001	22324 [†]	20
Caelo	Hydroquinone	15057001	22351 [†]	20
Caelo	Hydroquinone	16023105	23114	40
Caelo	Hydroquinone	172215	23654	40

- 126 692 spectra from a total of 2782 batches from further 781 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*.

- 209 spectra from 134 *Apo-Ident* customers from 58 batches from the substance/substance group *Hydroquinone*.

Supplier	Substance	Batch	Spectra
Caelo	Hydroquinone	1163902	1
Caelo	Hydroquinone	11163907	5
Caelo	Hydroquinone	11163905	4
Caelo	Hydroquinone	10145103	1
Caelo	Hydroquinone	11163912	4
Caesar & Loretz GmbH, 4. . .	Hydroquinone	11163912	1
Caelo	Hydroquinone	12156705	5
Caelo	Hydroquinone	14121202	1
Gehe	Hydroquinone	12156706	2
Caelo	Hydroquinone	20200712-3	1
Anzag	Hydroquinone	12156705	1
Caelo	Hydroquinone	1263912	1
Caelo	Hydroquinone	10145101	1
Caelo	Hydroquinone	12288505	11
Caelo	Hydroquinone	12156706	1
Caelo	Hydroquinone	1228503	1
Sanacorp	Hydroquinone	12288503	1
Caelo	Hydroquinone	12288502	2
Anzag	Hydroquinone	12288505	2
Phönix	Hydroquinone	12288503	2
Caelo	Hydroquinone	12288503	2
A.H. 14.06.13 ek: 3,97EUR	Hydroquinone	12288505	1
Sanacorp	Hydroquinone	12156703	1
Caelo	Hydroquinone	13105402	4
Caelo	Hydroquinone	11163912/Int312052	1
Caelo	Hydroquinone	13105405	6
Fagron	Hydroquinone		1
AHD	Hydroquinone	13105405	1
Caelo	Hydroquinone	10145113	2
Caelo	Hydroquinone	13105408	7
Caelo	Hydroquinone	18031403	1
Caesar & Loretz GmbH	Hydroquinone	13105405	1
Caelo	Hydroquinone	14026902	5
Phönix	Hydroquinone	13105408	1
14026902	Hydroquinone	InterneCharge1214Q	1
Caelo	Hydroquinone	14180401	3
Caelo	Hydroquinone	21102014A	1
Caelo	Hydroquinone	14180410	4
Caelo	Hydroquinone	14180406	3
Apomix/Noweda	Hydroquinone	13105408	1
Caelo	Hydroquinone	14281501	9
Phoenix Goettin	Hydroquinone	14281501	1
Caelo	Hydroquinone	14281507	4
Caelo	Hydroquinone	14280105	2
Caelo	Hydroquinone	16051502	1
Caelo	Hydroquinone	14280104	4
Caelo	Hydroquinone		2
Gehe/Gehe	Hydroquinone	14280110	1
ACM	Hydroquinone	KNC1047J15	2
Caelo	Hydroquinone	15057001	8
Caelo	Hydroquinone	15057004	9
Euro/Sanacorp	Hydroquinone	15057004	1
Caelo	Hydroquinone	1410401	1
Caelo	Hydroquinone	15057010	10
Caelo	Hydroquinone	15057002	1
Caelo	Hydroquinone	14026904	1
AHL	Hydroquinone	16023102	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydroquinone	16023105	10
phönix	Hydroquinone	16023105	1
Caelo	Hydroquinone	16023102	1
Sanacorp	Hydroquinone	16023103	1
Caeolo	Hydroquinone	16023105	1
Caelo	Hydroquinone	16023112	8
Caelo	Hydroquinone	52840166	1
GEHE	Hydroquinone	16023105	1
Caelo	Hydroquinone	15023105	1
Kehr	Hydroquinone	16023112	1
Caelo	Hydroquinone	4017A-01717	1
16023112	Hydroquinone	16023112	1
ACM	Hydroquinone	KNC0635J17	1
Caelo	Hydroquinone	16023113	4
Caelo	Hydroquinone	160231135430	1
Caeolo/Gehe	Hydroquinone	16023116	1
Caelo	Hydroquinone	16023116	10
Kehr	Hydroquinone	16023113	1
Allianz	Hydroquinone	16023116	1
Fiebig	Hydroquinone	16023116	1
Caelo	Hydroquinone	16023118	6
Caelo	Hydroquinone	20101806	1
Caelo	Hydroquinone	17221508	1

- 78 720 spectra from 565 *Apo-Ident* customers from a total of 26 081 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Hydroquinone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hydroquinone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 216
Type B	0	200	0	126 692
Type C	0	208	1	78 720

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8817 %)	99.5215 % (> 98.0861 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20884	21791	2.43	23.80
21468	21791	4.85	21.37
21791	21791	0.00	21.47
21923	21791	2.93	21.36
21975	21791	1.38	20.95
22324	21791	2.22	21.33
22351	21791	3.04	20.36

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Hydroxyethylcellulose (300 / 9000 mPa · s)
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20791-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydroxyethylcellulose (300 / 9000 mPa · s); Hydroxyethylcellulose (apparent viscosity 300 mPas); Hydroxyethylcellulose (apparent viscosity 9000 mPas); Hydroxyethylcellulose (nominal viscosity 300 mPas); Hydroxyethylcellulose (nominal viscosity 9000 mPas); Hydroxyethylcellulosum G 300; Hydroxyethylcellulosum HX

Special notes

When selecting the *Hydroxyethylcellulose (300 / 9000 mPa · s)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	European Pharmacopoeia 9th Edition, Basic Version 2017 [3]
Komm2.2.40	Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident [4]
AA004	Erstellung und Validierung eines IdentModul-Updates
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Hydroxyethylcellulose (300 / 9000 mPa · s)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydroxyethylcell...	12249204	20791	40	20120830
Euro OTC	Hydroxyethylcell...	1110024-04	20792	40	20120110

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydroxyethylcell...	03936475	20862	20	20121001
Fagron	Hydroxyethylcell...	13H22-N11	20908	40	20130826
Caelo	Hydroxyethylcell...	13378506	21365	40	1507205
Caelo	Hydroxyethylcell...	14352504	21792	40	AR-15-FG-009318-01
Caelo	Hydroxyethylcell...	161006	22459	40	20160426*
Fagron	Hydroxyethylcell...	16E09-B05-327042	23102	40	20160530
Caelo	Hydroxyethylcell...	16252008	23708	40	20160907
Caelo	Hydroxyethylcell...	16278705	23710	40	20161014

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 380 spectra of 10 reference samples from the substance/substance group *Hydroxyethylcellulose* (300 / 9000 mPa · s). These samples are listed above in the [calibration samples](#) section.
- 74116 spectra from a total of 1613 batches from further 371 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 10 reference samples from the substance/substance group *Hydroxyethylcellulose* (300 / 9000 mPa · s).

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydroxyethylcellulose (appar...	14352504	21792 [†]	20
Caelo	Hydroxyethylcellulose (appar...	161006	22459 [†]	20
Euro OTC	Hydroxyethylcellulose (appar...	1606030	22698	40
Caelo	Hydroxyethylcellulose (appar...	16012909	22809	40
Euro OTC	Hydroxyethylcellulose (appar...	1610039	22870	40
Caelo	Hydroxyethylcellulose (appar...	16252003	23584	40
Caelo	Hydroxyethylcellulose (appar...	16278705	23759	40
Caelo	Hydroxyethylcellulose (appar...	173196	23850	40
Euro OTC	Hydroxyethylcellulose (appar...	1711012	23904	40
Euro OTC	Hydroxyethylcellulose (appar...	1804003	24060	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.

- 126 532 spectra from a total of 2779 batches from further 780 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.

- 968 spectra from 347 *Apo-Ident* customers from 259 batches from the substance/substance group *Hydroxyethylcellulose (300 / 9000 mPa · s)*.

Supplier	Substance	Batch	Spectra
Fagron	Hydroxyethylcellulose (appar...	12A09-N06	2
Euro OTC	Hydroxyethylcellulose (appar...	1108026-01	2
Caelo	Hydroxyethylcellulose (appar...	11266305	1
Fagron	Hydroxyethylcellulose (appar...	12C27-N01	1
Euro OTC	Hydroxyethylcellulose (appar...	1406212528	1
Caelo	Hydroxyethylcellulose (appar...	12156901	1
Caelo	Hydroxyethylcellulose (appar...	12156902	1
Caelo	Hydroxyethylcellulose (appar...	11266316	1
Caelo	Hydroxyethylcellulose (appar...	1110024-01	1
Fagron	Hydroxyethylcellulose (appar...	11I02-N02	2
Euro OTC	Hydroxyethylcellulose (appar...	1105054-01	1
Euro OTC	Hydroxyethylcellulose (appar...	1110024-01	2
Euro OTC	Hydroxyethylcellulose (appar...	1108027-01	1
Euro OTC	Hydroxyethylcellulose (appar...	1110024-02	5
Fagron	Hydroxyethylcellulose (appar...	J0696	2
Fagron	Hydroxyethylcellulose (appar...	11I02-N12	1
Caelo	Hydroxyethylcellulose (appar...	12156907	9
Anzag	Hydroxyethylcellulose (appar...	1110024-03	3
Euro OTC	Hydroxyethylcellulose (appar...	1110024-03	17
Sanacorp	Hydroxyethylcellulose (appar...	12156901	1
Kehr	Hydroxyethylcellulose (appar...	211112PML01	1
Fagron	Hydroxyethylcellulose (appar...	12H02-N06	2
Gehe	Hydroxyethylcellulose (appar...	12156908	1
Caelo	Hydroxyethylcellulose (appar...	12156908	4
Caelo	Hydroxyethylcellulose (appar...	1110024-02	2
Caelo	Hydroxyethylcellulose (appar...	5012I-03301	1
Caelo	Hydroxyethylcellulose (appar...	213I-03301	1
Sanacorp	Hydroxyethylcellulose (appar...	1110024-03	1
Anzag	Hydroxyethylcellulose (appar...	12249204	1
Europharm/Otto	Hydroxyethylcellulose (appar...	1110024-03	1
Caelo	Hydroxyethylcellulose (appar...	19011302	1
s.Prüfprotokoll	Hydroxyethylcellulose (appar...		2
Caelo	Hydroxyethylcellulose (appar...	12249205	5
Caelo	Hydroxyethylcellulose (appar...	4512I-03301	1
Gehe	Hydroxyethylcellulose (appar...	13A18-N01	1
Fagron	Hydroxyethylcellulose (appar...	13A18-N01	4
Caelo	Hydroxyethylcellulose (appar...	11186221	1
Caelo	Hydroxyethylcellulose (appar...	1113E-03301	1
Caelo	Hydroxyethylcellulose (appar...	12249202	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	Hydroxyethylcellulose (appar...	20031305	1
EuRho	Hydroxyethylcellulose (appar...	1110024-03	1
Euro OTC	Hydroxyethylcellulose (appar...	111024-02	1
Caelo	Hydroxyethylcellulose (appar...	10019408	2
Euro OTC	Hydroxyethylcellulose (appar...	1110024-04	17
Caelo	Hydroxyethylcellulose (appar...	8051305	1
Caelo	Hydroxyethylcellulose (appar...	12369704	9
Caelo	Hydroxyethylcellulose (appar...	122492014	1
Europharm/Otto	Hydroxyethylcellulose (appar...	1110024-04	2
Holdermann	Hydroxyethylcellulose (appar...	1110024-04	1
Caelo	Hydroxyethylcellulose (appar...	12249216	5
Caelo	Hydroxyethylcellulose (appar...	1110024-04	1
Caelo	Hydroxyethylcellulose (appar...	12369713	2
Euro OTC	Hydroxyethylcellulose (appar...	130400801	1
Fagron	Hydroxyethylcellulose (appar...	13D26-N11	5
EuRho	Hydroxyethylcellulose (appar...	1110024-04	1
Caelo	Hydroxyethylcellulose (appar...	1304008-01	1
Euro OTC	Hydroxyethylcellulose (appar...	110505401	1
Phönix	Hydroxyethylcellulose (appar...	12369711	1
Caelo	Hydroxyethylcellulose (appar...	13153501	8
Caelo	Hydroxyethylcellulose (appar...	12249204	2
Caelo	Hydroxyethylcellulose (appar...	12369711	4
Noweda	Hydroxyethylcellulose (appar...	1108027-01	1
Euro OTC	Hydroxyethylcellulose (appar...	1304008-01	24
Caelo	Hydroxyethylcellulose (appar...	25071301	1
Euroo/Phoenix	Hydroxyethylcellulose (appar...	1304008-01	1
Caelo	Hydroxyethylcellulose (appar...	26071301	1
Caelo	Hydroxyethylcellulose (appar...	13153502	1
Ashland	Hydroxyethylcellulose (appar...	130400801	1
Sanacorp	Hydroxyethylcellulose (appar...	12H02-N06	1
Gehe	Hydroxyethylcellulose (appar...	111002404	1
Caelo	Hydroxyethylcellulose (appar...	12369717	1
Fagron	Hydroxyethylcellulose (appar...	13H22-N11	8
Euro OTC	Hydroxyethylcellulose (appar...	1110024-04-336431909	1
Euro OTC	Hydroxyethylcellulose (appar...	1304008-02	20
Caelo	Hydroxyethylcellulose (appar...	13153506	7
Phönix	Hydroxyethylcellulose (appar...	12369704	1
Euro OTC	Hydroxyethylcellulose (appar...	1007018-01	1
Caelo	Hydroxyethylcellulose (appar...	AKD10	1
Noweda	Hydroxyethylcellulose (appar...	13153501	1
Caelo	Hydroxyethylcellulose (appar...	12274720	1
Caelo	Hydroxyethylcellulose (appar...	13153505	10
Caelo	Hydroxyethylcellulose (appar...	1304008-02	2
Alliance Health 27.12.2...	Hydroxyethylcellulose (appar...	1304008-02	1
Caelo	Hydroxyethylcellulose (appar...	12369718	1
EuRho	Hydroxyethylcellulose (appar...	3081202	1
Caelo	Hydroxyethylcellulose (appar...	290114PML01	1
Euro OTC	Hydroxyethylcellulose (appar...	130400802	2
Caelo	Hydroxyethylcellulose (appar...	10019402	2
Caesar & Loretz GmbH	Hydroxyethylcellulose (appar...	13153501	1
Eurp	Hydroxyethylcellulose (appar...	130400801	2
Caelo	Hydroxyethylcellulose (appar...	13153511	7
Euro OTC	Hydroxyethylcellulose (appar...	1613M-03301	1
Gehe	Hydroxyethylcellulose (appar...	12369718	1
Euro OTC	Hydroxyethylcellulose (appar...	13040008-02	1
Caelo	Hydroxyethylcellulose (appar...	13378502	4
Euro OTC	Hydroxyethylcellulose (appar...	1309020-01	19
Caelo	Hydroxyethylcellulose (appar...	1309020-01	1
Caelo	Hydroxyethylcellulose (appar...	140317	1
Phonix	Hydroxyethylcellulose (appar...	1309020-01	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Hydroxyethylcellulose (appar...	K1371	2
Caelo	Hydroxyethylcellulose (appar...	1315306	1
Caelo	Hydroxyethylcellulose (appar...	31031402	1
Fagron	Hydroxyethylcellulose (appar...	1309020-01	1
Euro OTC	Hydroxyethylcellulose (appar...	130902001	1
Euro OTC	Hydroxyethylcellulose (appar...	17042014A	1
Caelo	Hydroxyethylcellulose (appar...	13378508	3
Fagron	Hydroxyethylcellulose (appar...	13L04-B03-289115	1
Ashland/Sanacorp	Hydroxyethylcellulose (appar...	1309020-01	1
Caelo	Hydroxyethylcellulose (appar...	19051406	1
Caelo	Hydroxyethylcellulose (appar...	13378507	9
Nachprüfung	Hydroxyethylcellulose (appar...	13d26-n16	2
Caelo	Hydroxyethylcellulose (appar...	130902001	1
Fagron	Hydroxyethylcellulose (appar...	13L04-B03	1
AHD	Hydroxyethylcellulose (appar...	13153511	1
Euro OTC	Hydroxyethylcellulose (appar...	1309020-02	5
Euro OTC	Hydroxyethylcellulose (appar...	12175708	1
Alliance Healthcare/Hed...	Hydroxyethylcellulose (appar...	1309020-02	1
	Hydroxyethylcellulose (appar...	1304008-01	1
Euro OTC	Hydroxyethylcellulose (appar...	1309020-03	9
Phoenix 10.07.2014	Hydroxyethylcellulose (appar...	1309020-01	1
Caelo	Hydroxyethylcellulose (appar...	213M-03301	1
Th. Geyer	Hydroxyethylcellulose (appar...	13L04-B03	1
Phönix	Hydroxyethylcellulose (appar...	13L04-B03-289115	2
Caelo	Hydroxyethylcellulose (appar...	13378515	3
Caelo	Hydroxyethylcellulose (appar...	10019406	2
Caelo	Hydroxyethylcellulose (appar...	1406017-01	3
Sanacorp/Phoenix	Hydroxyethylcellulose (appar...	1309020-01	1
Gehe 24.06.2014	Hydroxyethylcellulose (appar...	13153505	1
Euro OTC	Hydroxyethylcellulose (appar...	13099020-01	1
Noweda	Hydroxyethylcellulose (appar...	13378507	1
Caelo	Hydroxyethylcellulose (appar...	1337808	1
Caelo	Hydroxyethylcellulose (appar...	220914PML02	1
Fagron	Hydroxyethylcellulose (appar...	14f04-b06-295130	1
Fagron	Hydroxyethylcellulose (appar...	K1373	2
Defektur	Hydroxyethylcellulose (appar...	1309020-01	1
Fagron	Hydroxyethylcellulose (appar...	14D04-B02	2
Euro OTC	Hydroxyethylcellulose (appar...	1406017-01	32
Fagron	Hydroxyethylcellulose (appar...	14D04B02293555	1
Fagron	Hydroxyethylcellulose (appar...	14F04-B06-295130	1
Caelo	Hydroxyethylcellulose (appar...	1337807	1
Caesar/Noweda	Hydroxyethylcellulose (appar...	13378507	1
Euro OTC	Hydroxyethylcellulose (appar...	914E-03301	1
Caelo	Hydroxyethylcellulose (appar...	21011502	1
Caelo	Hydroxyethylcellulose (appar...	13378506	3
Euro OTC	Hydroxyethylcellulose (appar...	130902003	1
Euro OTC	Hydroxyethylcellulose (appar...	1406017	1
Caelo	Hydroxyethylcellulose (appar...	1309020	1
Phoenix Goettin	Hydroxyethylcellulose (appar...	14F04-B06-295130	1
Caelo	Hydroxyethylcellulose (appar...	13041502	1
Fagron	Hydroxyethylcellulose (appar...	14I04-B05	1
Fagron	Hydroxyethylcellulose (appar...	14I04-B05-300224	2
Caelo	Hydroxyethylcellulose (appar...	13378516	2
Caelo	Hydroxyethylcellulose (appar...	14256002	2
Caelo	Hydroxyethylcellulose (appar...	13378518	3
Gehe	Hydroxyethylcellulose (appar...	1406017-01	1
Fagron	Hydroxyethylcellulose (appar...	14D04-B02-293558	2
Caelo	Hydroxyethylcellulose (appar...	13378510	2
Euro OTC	Hydroxyethylcellulose (appar...	1406017-02	36
Noweda	Hydroxyethylcellulose (appar...	13153511	1

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Supplier	Substance	Batch	Spectra
Fagron	Hydroxyethylcellulose (appar...	1404-B05-300231	1
Fagron	Hydroxyethylcellulose (appar...	14I04-B05-300231	2
Caelo	Hydroxyethylcellulose (appar...	15086405	8
Fagron	Hydroxyethylcellulose (appar...	14I04-B05	1
Caelo	Hydroxyethylcellulose (appar...	13378524	1
Caelo	Hydroxyethylcellulose (appar...	15086403	3
EuRho/GEHE	Hydroxyethylcellulose (appar...	1309020-03	1
Euro OTC	Hydroxyethylcellulose (appar...	1496017-02	1
Euro OTC	Hydroxyethylcellulose (appar...	13072015A	1
Caelo	Hydroxyethylcellulose (appar...	15086407	5
Nachprüfung 2797	Hydroxyethylcellulose (appar...	12249202	1
Fagron	Hydroxyethylcellulose (appar...	15086407	1
Caelo	Hydroxyethylcellulose (appar...	1406017-02	3
Euro OTC	Hydroxyethylcellulose (appar...	140601702	1
Caelo	Hydroxyethylcellulose (appar...	15086408	1
Fagron	Hydroxyethylcellulose (appar...	15086403	1
Fagron	Hydroxyethylcellulose (appar...	14I04-B05-309049	1
Phönix	Hydroxyethylcellulose (appar...	1406017-02	1
Caelo	Hydroxyethylcellulose (appar...	133785	1
Fagron	Hydroxyethylcellulose (appar...	1406017-02	2
Euro OTC	Hydroxyethylcellulose (appar...	1504018-01	15
Fagron	Hydroxyethylcellulose (appar...	14i04-b05-309049	1
Caelo	Hydroxyethylcellulose (appar...	15086505	1
Caelo	Hydroxyethylcellulose (appar...	140601701	1
Caelo	Hydroxyethylcellulose (appar...	15086506	1
Euro OTC	Hydroxyethylcellulose (appar...	1504018-02	26
Caelo	Hydroxyethylcellulose (appar...	15086504	2
Ashland Industries/Anzag	Hydroxyethylcellulose (appar...	L1891	1
Fagron	Hydroxyethylcellulose (appar...	15B04-B03-312859	3
Caelo	Hydroxyethylcellulose (appar...	15086503	1
Fagron	Hydroxyethylcellulose (appar...	1504018-02	1
Caelo	Hydroxyethylcellulose (appar...	1504018-1	1
Castor/Phönix	Hydroxyethylcellulose (appar...	1504018-01	1
Fagron	Hydroxyethylcellulose (appar...	14/04-B05-300231	1
Fagron	Hydroxyethylcellulose (appar...	15B04-B03-315495	1
Euro OTC	Hydroxyethylcellulose (appar...	154018-02	1
Fagron	Hydroxyethylcellulose (appar...	14F04-B06-297846	1
Caelo	Hydroxyethylcellulose (appar...	15086507	1
Euro OTC	Hydroxyethylcellulose (appar...	1504018-03	21
Fagron	Hydroxyethylcellulose (appar...	15E07-B05-316511	2
Caelo	Hydroxyethylcellulose (appar...	1504018-02	3
Fagron	Hydroxyethylcellulose (appar...	15H28-B10	2
Caelo	Hydroxyethylcellulose (appar...	16100606	15
Caelo	Hydroxyethylcellulose (appar...	140601702	1
Euro OTC	Hydroxyethylcellulose (appar...	80616-3	1
Fagron	Hydroxyethylcellulose (appar...	15H28-B10-319028	2
phönix	Hydroxyethylcellulose (appar...	15e07b05316511	1
Euro OTC	Hydroxyethylcellulose (appar...	150401801	1
Caelo	Hydroxyethylcellulose (appar...	1504018-03	1
Caelo	Hydroxyethylcellulose (appar...	16100612	2
Caelo	Hydroxyethylcellulose (appar...	16100613	2
Euro OTC	Hydroxyethylcellulose (appar...	1406017-03	2
Euro OTC	Hydroxyethylcellulose (appar...	3081603	1
Ebert & Jacobi 02.08.2016	Hydroxyethylcellulose (appar...	16100606	1
Euro OTC	Hydroxyethylcellulose (appar...	1504019-02	1
Euro OTC	Hydroxyethylcellulose (appar...	1500418-02	1
Ashland Ind/Gehe	Hydroxyethylcellulose (appar...	140017-01	1
Phönix	Hydroxyethylcellulose (appar...	16100606	1
Caelo	Hydroxyethylcellulose (appar...	1606030-01	7
Caelo	Hydroxyethylcellulose (appar...	16100607	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydroxyethylcellulose (appar...	16100604	2
Euro OTC	Hydroxyethylcellulose (appar...	1606030-01	31
Caelo	Hydroxyethylcellulose (appar...	16100605	2
Fagron	Hydroxyethylcellulose (appar...	16E09-B05-321320	2
Caelo	Hydroxyethylcellulose (appar...	16100615	4
Caelo	Hydroxyethylcellulose (appar...	160603001	1
Caelo	Hydroxyethylcellulose (appar...	16100620	3
Caelo	Hydroxyethylcellulose (appar...	16100617	8
Euro OTC	Hydroxyethylcellulose (appar...	1606030-02	19
apo-ident.	Hydroxyethylcellulose (appar...	1606030-02	1
Caelo	Hydroxyethylcellulose (appar...	16100610	3
Caelo	Hydroxyethylcellulose (appar...	16100622	4
Fagron	Hydroxyethylcellulose (appar...	16H05B05325803	1
hedinger	Hydroxyethylcellulose (appar...	1606030	1
Euro OTC	Hydroxyethylcellulose (appar...	16060302-02	1
Euro OTC	Hydroxyethylcellulose (appar...	16603001	1
Anzag	Hydroxyethylcellulose (appar...	1606030-02	1
apo ident	Hydroxyethylcellulose (appar...	1606030-02	1
Fagron	Hydroxyethylcellulose (appar...	16H05-B05	1
Caelo	Hydroxyethylcellulose (appar...	16100625	13
Fagron	Hydroxyethylcellulose (appar...	16107-b04-331244	1
Euro OTC	Hydroxyethylcellulose (appar...	1610039-01	30
Fagron	Hydroxyethylcellulose (appar...	16E09-B05-327042	1
Caelo	Hydroxyethylcellulose (appar...	16100603	1
Fagron	Hydroxyethylcellulose (appar...	16L07-B04-331244	2
Caelo	Hydroxyethylcellulose (appar...	19041708	1
Fiebig	Hydroxyethylcellulose (appar...	1606030-02	1
Caelo	Hydroxyethylcellulose (appar...	16100626	6
Euro OTC	Hydroxyethylcellulose (appar...	N1535	1
gepepharm/Phönix	Hydroxyethylcellulose (appar...	160603002	1
Gehe	Hydroxyethylcellulose (appar...	16100617	1
Noweda	Hydroxyethylcellulose (appar...	1309020-03	1
Fagron	Hydroxyethylcellulose (appar...	16L07-B04-331846	2
Caelo	Hydroxyethylcellulose (appar...	16278702	2
Euro OTC	Hydroxyethylcellulose (appar...	160603	1
Caelo	Hydroxyethylcellulose (appar...	1610039-01	2
Alliance Healthcare	Hydroxyethylcellulose (appar...	16L07-B04-331846	1
Caelo	Hydroxyethylcellulose (appar...	19081705	1
Euro/Sanacorp	Hydroxyethylcellulose (appar...	1610039-01	4
GEHE	Hydroxyethylcellulose (appar...	1610039-01	2
phönix	Hydroxyethylcellulose (appar...	1610039-02	1
Fagron	Hydroxyethylcellulose (appar...	16H05-B05-325803	1
Caelo	Hydroxyethylcellulose (appar...	16278705	7
Caelo	Hydroxyethylcellulose (appar...	1606030-03	1
Euro OTC	Hydroxyethylcellulose (appar...	1610039-02	3
Caelo	Hydroxyethylcellulose (appar...	1610039-02	1
Caelo	Hydroxyethylcellulose (appar...	27101701	1
Euro OTC	Hydroxyethylcellulose (appar...	1610036-01	1
Euro OTC	Hydroxyethylcellulose (appar...	1610039-03	6
Caelo	Hydroxyethylcellulose (appar...	16278715	2
Fagron	Hydroxyethylcellulose (appar...	17G05-B04-341204	5
Caelo	Hydroxyethylcellulose (appar...	11121707	1
Euro OTC	Hydroxyethylcellulose (appar...	160039-01	1
Euro OTC	Hydroxyethylcellulose (appar...	1711012-01	19
Euro OTC	Hydroxyethylcellulose (appar...	1606030-03	1
Sanacorp	Hydroxyethylcellulose (appar...	16278705	1
Euro OTC	Hydroxyethylcellulose (appar...	180201HC/1610039-01	1
Fagron	Hydroxyethylcellulose (appar...	17G05-B04	3
Caelo	Hydroxyethylcellulose (appar...	17G05-B04-341204	2
Caelo	Hydroxyethylcellulose (appar...	16278718	2

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Supplier	Substance	Batch	Spectra
Euro OTC	Hydroxyethylcellulose (appar...	171101201	2
Caelo	Hydroxyethylcellulose (appar...	16278714	4
Kehr	Hydroxyethylcellulose (appar...	16278718	1
Caelo	Hydroxyethylcellulose (appar...	12031803	1
Caelo	Hydroxyethylcellulose (appar...	18022401	2
Caelo	Hydroxyethylcellulose (appar...	23041804	1
Caelo	Hydroxyethylcellulose (appar...	1610039-03	1
Caelo	Hydroxyethylcellulose (appar...	1711012-01	1
Caelo	Hydroxyethylcellulose (appar...	17J05-B03-342018	1
Kehr/ Ashland Industries	Hydroxyethylcellulose (appar...	1711012-01	2
Hepart	Hydroxyethylcellulose (appar...	1606030-01	1
Fagron	Hydroxyethylcellulose (appar...	17j05B03342018	1
Ashland Industries/ All...	Hydroxyethylcellulose (appar...	1711012-01	1
Fagron	Hydroxyethylcellulose (appar...	1711012-01	1
Caelo	Hydroxyethylcellulose (appar...	23061809	1
Euro OTC	Hydroxyethylcellulose (appar...	161003901	1
Caelo	Hydroxyethylcellulose (appar...	21071802	1
Fagron	Hydroxyethylcellulose (appar...	17J05-B03-347890	5
Henry Lamotte/ Noweda	Hydroxyethylcellulose (appar...	1711012-01	1
Caelo	Hydroxyethylcellulose (appar...	12091819	1
Caelo	Hydroxyethylcellulose (appar...	17319602	1
Euro OTC	Hydroxyethylcellulose (appar...	P0745	1
Caelo	Hydroxyethylcellulose (appar...	21111812	1
phoenix 23.11.18	Hydroxyethylcellulose (appar...	1711012-01	1
Euro OTC	Hydroxyethylcellulose (appar...	1711012	1
Caelo	Hydroxyethylcellulose (appar...	17Jo5-B03-343927	1
Caelo	Hydroxyethylcellulose (appar...	12011903	1
Caelo	Hydroxyethylcellulose (appar...	17319603	1
fargon GmbH	Hydroxyethylcellulose (appar...	18C05-B05-352498	1
Caelo	Hydroxyethylcellulose (appar...	11304620	4
Euro OTC	Hydroxyethylcellulose (appar...	11110024-03	1
Caesar & Loretz GmbH D...	Hydroxyethylcellulose (appar...	12274702	1
Caelo	Hydroxyethylcellulose (appar...	12274710	2
Caelo	Hydroxyethylcellulose (appar...	13182702	6
Euro OTC	Hydroxyethylcellulose (appar...	314Q3301	1
Phönix	Hydroxyethylcellulose (appar...	1304008-02	1
Caelo	Hydroxyethylcellulose (appar...	13182714	1
Caelo	Hydroxyethylcellulose (appar...	1309020-01	1
Gutenberg-Apotheke	Hydroxyethylcellulose (appar...	11048105	1
Euro OTC	Hydroxyethylcellulose (appar...	1406017-01	1
Caelo	Hydroxyethylcellulose (appar...	14095905	1
Fagron	Hydroxyethylcellulose (appar...	130902002	1
Caelo	Hydroxyethylcellulose (appar...	14095911	3
Caelo	Hydroxyethylcellulose (appar...	12274702	1
Caelo	Hydroxyethylcellulose (appar...	14352508	1
Caelo	Hydroxyethylcellulose (appar...	14352510	4
Caelo	Hydroxyethylcellulose (appar...	14095901	1
Fagron	Hydroxyethylcellulose (appar...	14352504	1
Bombastus	Hydroxyethylcellulose (appar...	14095911	1
Euro OTC	Hydroxyethylcellulose (appar...	146017-02	1
Caelo	Hydroxyethylcellulose (appar...	15199501	8
Jenne	Hydroxyethylcellulose (appar...	15199501	1
Euro OTC	Hydroxyethylcellulose (appar...	1504018-03	1
Caelo	Hydroxyethylcellulose (appar...	16100606	1
Euro OTC	Hydroxyethylcellulose (appar...	16012909	1
Caelo	Hydroxyethylcellulose (appar...	16012909	5
Caelo	Hydroxyethylcellulose (appar...	16252003	1
Caelo	Hydroxyethylcellulose (appar...	16012901	1
Caelo	Hydroxyethylcellulose (appar...	16252006	5
Rezepturlager - Verläng...	Hydroxyethylcellulose (appar...	54/16	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydroxyethylcellulose (appar...	4091713	1
Caelo	Hydroxyethylcellulose (appar...	16091711	1
Caelo	Hydroxyethylcellulose (appar...	16252008	2
Caelo	Hydroxyethylcellulose (appar...	5121706	1
Caelo	Hydroxyethylcellulose (appar...	17184503	7
Caelo	Hydroxyethylcellulose (appar...	9041802	1
Caelo	Hydroxyethylcellulose (appar...	18022502	1
Caelo	Hydroxyethylcellulose (appar...	9061802	1
Caelo	Hydroxyethylcellulose (appar...	18022503	1
Caelo	Hydroxyethylcellulose (appar...	18113101	1
Caelo	Hydroxyethylcellulose (appar...	18022507	2
Caelo	Hydroxyethylcellulose (appar...	17101801	1
Caelo	Hydroxyethylcellulose (appar...	28111804	1
Caelo	Hydroxyethylcellulose (appar...	28111805	1
Caelo	Hydroxyethylcellulose (appar...	23011901	1

- 77 961 spectra from 565 *Apo-Ident* customers from a total of 25 885 batches from a further 692 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Hydroxyethylcellulose (300 / 9000 mPa · s)* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hydroxyethylcellulose (300 / 9000 mPa · s)* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	380	0	74 116
Type B	0	360	0	126 459
Type C	0	963	5	77 961

The substance/substance group *Hydroxyethylcellulose (300 / 9000 mPa · s)* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.8817 %)	99.4835 % (> 99.1736 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20862	22459	9.28	55.62
21792	21792	0.00	58.00
23708	21792	2.97	57.40
20791	21365	15.47	55.14
20792	21792	13.54	53.84
20908	21365	17.29	52.66
21365	21365	0.00	56.36
22459	22459	0.00	56.77
23102	21792	9.33	56.16
23710	21792	11.75	55.44

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Hydroxypropylcellulose (300 mPa · s)**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20686-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hydroxypropylcellulose (300 mPa · s); Hydroxypropylcellulosum (300 mPa · s)

Special notes

When selecting the *Hydroxypropylcellulose (300 mPa · s)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Hydroxypropylcellulose (300 mPa · s)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydroxypropylcel...	12093107	20686	40	1402049
Caelo	Hydroxypropylcel...	14189804	21767	40	AR-15-FG-014922-01
Caelo	Hydroxypropylcel...	15345001	22258	40	20151104
Caelo	Hydroxypropylcel...	181146	24249	40	20180618*

Validation samples

A total of 280 317 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 *Hydroxypropylcellulose* (300 mPa · s). These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Hydroxypropylcellulose* (300 mPa · s).

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydroxypropylcellulose (300 ...	14189804	21767 [†]	20
Caelo	Hydroxypropylcellulose (300 ...	15345001	22258 [†]	20
Caelo	Hydroxypropylcellulose (300 ...	15345009	23123	40
Caelo	Hydroxypropylcellulose (300 ...	17355801	23974	40

- 126 772 spectra from a total of 2785 batches from further 781 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*.

- 6 spectra from 6 *Apo-Ident* customers from 6 batches from the substance/substance group *Hydroxypropylcellulose (300 mPa · s)*.

Supplier	Substance	Batch	Spectra
Caelo	Hydroxypropylcellulose (300 ...	13031306	1
Caelo	Hydroxypropylcellulose (300 ...	14189801	1
Caelo	Hydroxypropylcellulose (300 ...	13031309	1
Caelo	Hydroxypropylcellulose (300 ...	15345001	1
Caelo	Hydroxypropylcellulose (300 ...	15129707	1
Caelo	Hydroxypropylcellulose (300 ...	15345008	1

- 78 923 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Hydroxypropylcellulose (300 mPa · s)* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hydroxypropylcellulose (300 mPa · s)* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	119	1	126 772
Type C	0	5	1	78 923

The substance/substance group *Hydroxypropylcellulose (300 mPa · s)* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	99.1667 % (> 96.6667 %)
Type C	100.0000 % (> 99.8819 %)	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
20686	20686	0.00	21.69
21767	21767	0.00	22.81
22258	21767	9.62	27.10
24249	24249	0.00	20.65

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Hyoscine butylbromide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20766-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hyoscine butylbromide; Hyoscini butylbromidum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Hyoscine butylbromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Hyoscine butylbr...	12K01-N07	20766	40	1406057
Fagron	Hyoscine butylbr...	12K01-N07	20897	40	20121102
Fagron	Hyoscine butylbr...	13K22-N03	21049	40	20131126
Fagron	Hyoscine butylbr...	15I09-B04-312245	21954	40	20150921
Fagron	Hyoscine butylbr...	15I09-B04-316806	22344	40	20150921

Validation samples

A total of 280 317 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 *Hyoscine butylbromide*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1619 batches from further 372 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 *Hyoscine butylbromide*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Hyoscine butylbromide	15I09-B04-312245	21954 [†]	20
Fagron	Hyoscine butylbromide	15I09-B04-316806	22344 [†]	20
Fagron	Hyoscine butylbromide	16I20-B08-326942	22903	40
Fagron	Hyoscine butylbromide	16I20-B08-326942	22937	40

- 126 772 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 12 spectra from 4 *Apo-Ident* customers from 1 batches from the substance/substance group *Hyoscine butylbromide*.

[†]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
Fagron	Hyoscine butylbromide	16I20-B08-326942	12

- 78 917 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Hyoscine butylbromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hyoscine butylbromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	120	0	126 772
Type C	0	12	0	78 917

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8818 %)	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
20766	20766	0.00	85.56
20897	20766	14.77	87.76
21049	20766	5.36	86.89
21954	20766	5.81	87.26
22344	20766	5.86	87.52

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Hyoscine hydrobromide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21676-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hyoscine hydrobromide; Scopolamini hydrobromidum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Hyoscine hydrobromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hyoscine hydrobr...	14278801	21676	40	1504154
Caelo	Hyoscine hydrobr...	15054501	21764	40	1511156
Fagron	Hyoscine hydrobr...	15L09-B04-334706	23418	40	20151228
Fagron	Hyoscine hydrobr...	15L09-B04-334706	23419	40	20151228
Caelo	Hyoscine hydrobr...	15054501	21764SI	28	1511156

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 188 spectra of 5 reference samples from the substance/substance group *Hyoscine hydrobromide*. These samples are listed above in the [calibration samples](#) section.
- 74 308 spectra from a total of 1620 batches from further 372 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 [†].

- 322 spectra of 9 reference samples from the substance/substance group *Hyoscine hydrobromide*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hyoscine hydrobromide	14278801	21676 [†]	20
Caelo	Hyoscine hydrobromide	15054501	21764 [†]	20
Caelo	Hyoscine hydrobromide	15054504	21925	60
Caelo	Hyoscine hydrobromide	15054504	23441	40
Caelo	Hyoscine hydrobromide	15054501	21764SI [†]	32
Caelo	Hyoscine hydrobromide	15054504	21925SI	30
Fagron	Hyoscine hydrobromide	15L09-B04-334706	23418SI	40
Fagron	Hyoscine hydrobromide	15L09-B04-334706	23419SI	40
Caelo	Hyoscine hydrobromide	15054504	23441SI	40

- 126 570 spectra from a total of 2785 batches from further 781 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*.

- 30 spectra from 9 *Apo-Ident* customers from 5 batches from the substance/substance group *Hyoscine hydrobromide*.

Supplier	Substance	Batch	Spectra
Fagron	Hyoscine hydrobromide	14J27-B05-307020	1
Caelo	Hyoscine hydrobromide	15358901	1
Caelo	Hyoscine hydrobromide	14278801	26
Caelo	Hyoscine hydrobromide	15054505	1
Caelo	Hyoscine hydrobromide	16206204	1

- 78 899 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	188	0	74 308
Type B	0	287	35	126 570
Type C	0	29	1	78 899

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.8085 %)
Type B	100.0000 % (> 99.9901 %)	89.1304 % (> 88.1988 %)
Type C	100.0000 % (> 99.8817 %)	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
21764	21764	0.00	26.11
23418	21764	7.99	23.89
23419	21764	5.49	23.39
21676	21676	0.00	20.57

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ibuprofen**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20205-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ibuprofen; Ibuprofenum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ibuprofen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ibuprofen	11352219	20774	40	20120124
Euro OTC	Ibuprofen	1211011-02	21248	40	1501533
Caelo	Ibuprofen	172271	23641	40	20170831*

Validation samples

A total of 280 317 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 *Ibuprofen*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Ibuprofen*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ibuprofen	13105108	21321	40
Euro OTC	Ibuprofen	1410025-02	23587	40

- 126 812 spectra from a total of 2787 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 20 spectra from 10 *Apo-Ident* customers from 9 batches from the substance/substance group *Ibuprofen*.

Supplier	Substance	Batch	Spectra
Euro OTC	Ibuprofen	1211011-01	1
Euro OTC	Ibuprofen	1410025-01	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
Euro OTC	Ibuprofen	1410025-02	6
Caelo	Ibuprofen	1410025-02	1
Caelo	Ibuprofen		1
GEHE	Ibuprofen	15103011	1
Caelo	Ibuprofen	17227101	1
Caelo	Ibuprofen	17227102	1
Euro OTC	Ibuprofen	9061807	1
Caelo	Ibuprofen	17351401	1

- 78 909 spectra from 565 *Apo-Ident* customers from a total of 26 128 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ibuprofen* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ibuprofen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	80	0	126 812
Type C	0	18	2	78 909

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8817 %)	90.0000 % (> 75.0000 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20774	21248	8.32	50.05
21248	21248	0.00	37.21
23641	23641	0.00	41.86

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Indometacin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20720-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Indometacin; Indometacinum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Indometacin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Indometacin	1012009-02	20720	40	1402050
Euro OTC	Indometacin	1205002-01	21327	40	20120521
Euro OTC	Indometacin	1512031	22291	40	20160122*
Euro OTC	Indometacin	1612017	22981	40	20170209*

Validation samples

A total of 280317 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 *Indometacin*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 *Indometacin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Indometacin	1512031	22291 [†]	20
Fagron	Indometacin	17I08-B06-339738	23715	40
Euro OTC	Indometacin	1801040	23969	40

- 126792 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 18 spectra from 14 *Apo-Ident* customers from 9 batches from the substance/substance group *Indometacin*.

*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	Indometacin	1205002-01	2
Euro OTC	Indometacin	1512031-01	4
Fagron	Indometacin		1
Gehe	Indometacin	1512031-01	1
Euro OTC	Indometacin	1612017-02	3
Fagron	Indometacin	17I08-B06-339738	1
Euro OTC	Indometacin	1801040-01	3
Fagron	Indometacin	14I08-B06-343286	1
Euro OTC	Indometacin	201606272030	1
Euro OTC	Indometacin	180104001	1

- 78 911 spectra from 565 *Apo-Ident* customers from a total of 26 129 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Indometacin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Indometacin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	100	0	126 792
Type C	0	17	1	78 911

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
20720	20720	0.00	67.90
21327	20720	4.52	68.85
22291	22291	0.00	68.95
22981	22981	0.00	67.82

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Inositol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20420-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Inositol; Inositolium

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Inositol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Inositol	1206032-01	21280	40	20120814
Fagron	Inositol	13D15-B40-328250	23406	40	AR-17-FG-016393-01

Validation samples

A total of 280 317 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 *Inositol*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Inositol*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Inositol	L1507021-01	22797	40
Fagron	Inositol	13D15-B40-328250	23405	40
Fagron	Inositol	18A03-B04-344527	23999	40

- 126 772 spectra from a total of 2786 batches from further 781 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 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Inositol*.

Supplier	Substance	Batch	Spectra
Euro OTC	Inositol	130400901	1
Fagron	Inositol	L13090200	1
Euro OTC	Inositol	1609025-01	1
Euro OTC	Inositol	1304009-01	1
Caelo	Inositol	L1609025-01	1

- 78 924 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Inositol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Inositol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	120	0	126 772
Type C	0	5	0	78 924

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8819 %)	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
21280	23406	4.10	36.21
23406	23406	0.00	36.50

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Iodoform
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20094-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Iodoform; Iodoformium

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Iodoform*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Iodoform	12L11-B41	21278	40	20140113
Caelo	Iodoform	12283206	21297	40	20130709
Caelo	Iodoform	16012302	23192	40	AR-17-FG-012459-01

Validation samples

A total of 280 317 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 *Iodoform*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 4 reference samples from the substance/substance group *Iodoform*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Iodoform	16012302	23407	40
Caelo	Iodoform	170860	23652	30
Caelo	Iodoform	180919	24012	40
Caelo	Iodoform	182495	24380	40

- 126 742 spectra from a total of 2785 batches from further 781 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.

- 222 spectra from 94 *Apo-Ident* customers from 85 batches from the substance/substance group *Iodoform*.

Supplier	Substance	Batch	Spectra
Caelo	Iodoform	12070102	2
Noweda	Iodoform	10320402	1
Noweda	Iodoform	12070407	1

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Supplier	Substance	Batch	Spectra
Caelo	Iodoform	12070502	1
Caelo	Iodoform	12070605	1
Caelo	Iodoform	12070501	1
Caelo	Iodoform	12070602	1
Fagron	Iodoform	12E30-N01	2
Caelo	Iodoform	12150902	5
Caelo	Iodoform	12150903	1
Caelo	Iodoform	12070606	2
Caelo	Iodoform	21051305	1
Phoenix	Iodoform	12070601	1
Caelo	Iodoform	12070608	3
Caelo	Iodoform	12070407	1
Caelo	Iodoform	12150905	2
Caelo	Iodoform	12150908	4
Caelo	Iodoform	12070601	2
Caelo	Iodoform	12283202	5
Caelo	Iodoform	12150910	4
Caelo	Iodoform	12283201	2
Caelo	Iodoform	12283206	3
Fagron	Iodoform	12L11-B41-290055	1
Caelo	Iodoform	14077702	7
Caelo	Iodoform	14077603	2
Caelo	Iodoform	12283304	1
Caelo	Iodoform	14077601	1
Caelo	Iodoform	12283303	1
Caelo	Iodoform	14077606	2
Caelo	Iodoform	14229507	2
Caelo	Iodoform	14077607	1
Caelo	Iodoform	14230001	5
Caelo	Iodoform	14230002	2
Caelo	Iodoform	14229508	2
Caelo	Iodoform	14230006	4
Caelo	Iodoform	14230007	3
Caelo	Iodoform	14230003	1
Caelo	Iodoform	14230008	3
Fagron	Iodoform	14229508	1
Caelo	Iodoform	14230302	2
Caelo	Iodoform	14077602	1
Gehe	Iodoform	14230008	1
Caelo	Iodoform	14230305	7
Euro OTC	Iodoform	14229504	2
Caelo	Iodoform	14230306	4
Caelo	Iodoform	14230308	4
Caelo	Iodoform	15276102	5
Caelo	Iodoform	15276001	3
Caelo	Iodoform	15276002	3
Caelo	Iodoform	15276101	5
Caelo	Iodoform	15276104	3
Caelo	Iodoform	1010316	1
Caelo	Iodoform	15276105	6
Caelo	Iodoform	15276103	4
Caelo	Iodoform	1576103	1
Caelo	Iodoform	15276108	2
Caelo	Iodoform	15276111	5
Caelo	Iodoform	15276107	1
Caelo	Iodoform	1527104	1
Caelo	Iodoform	15276109	1
Caelo	Iodoform	1527611	1
Caelo	Iodoform	16012201	5
Caelo	Iodoform	14230304	2

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Supplier	Substance	Batch	Spectra
Caelo	Iodoform	16012205	2
Caelo	Iodoform	16012206	4
Caelo	Iodoform	16012204	3
Caelo	Iodoform	16012202	2
Caelo	Iodoform	16012305	3
Caelo	Iodoform	16012207	3
Caelo	Iodoform	15276113	1
Caelo	Iodoform	16012210	4
Caelo	Iodoform	16012309	3
Caesar u.Loretz	Iodoform	16012209	2
Caelo	Iodoform	16012302	2
Caelo	Iodoform	12070105	1
Caelo	Iodoform	16012306	5
Caelo	Iodoform	16012308	2
Caelo	Iodoform	17086008	3
Caelo	Iodoform	17086005	4
GEHE	Iodoform	17086003	1
Sanacorp	Iodoform	17086005	1
Caelo	Iodoform	17086004	2
Caelo	Iodoform	17086006	5
Caelo	Iodoform	18091802	2
Caelo	Iodoform	17086002	1
Caelo	Iodoform	18091805	5
Fagron	Iodoform	18091803	1
Caelo	Iodoform	18091806	1
Caelo	Iodoform	18091804	3
Caelo	Iodoform	18091801	1

- 78 707 spectra from 565 *Apo-Ident* customers from a total of 26 053 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Iodoform* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Iodoform* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	150	0	126 742
Type C	0	219	3	78 707

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.8817 %)	98.6486 % (> 97.2973 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21278	23192	10.90	94.07
21297	23192	15.54	96.36
23192	23192	0.00	90.59

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Ipratropium bromide
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20911-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ipratropium bromide; Ipratropii bromidum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

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

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

Finally, 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 *Ipratropium bromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ipratropium brom...	12C15-N01	20911	40	1403675
Fagron	Ipratropium brom...	12K01-N08	21272	40	20121025

Validation samples

A total of 280 317 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 *Ipratropium bromide*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Ipratropium bromide*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ipratropium bromide	15C04-B02-321674	22747	40
Fagron	Ipratropium bromide	16K07-B05-335330	23597	40
Fagron	Ipratropium bromide	18B19-B05-346997	23992	40

- 126 772 spectra from a total of 2786 batches from further 781 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 *Ipratropium bromide*.

Supplier	Substance	Batch	Spectra
Fagron	Ipratropium bromide	14B05-B16-294566	1

- 78 928 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ipratropium bromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ipratropium bromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	119	1	126 772
Type C	0	1	0	78 928

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	99.1667 % (> 96.6667 %)
Type C	100.0000 % (> 99.8830 %)	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
20911	20911	0.00	49.11
21272	20911	2.56	47.37

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Isosorbide dinitrate 40%**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20213-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Isosorbide dinitrate 40%; Isorbidi dinitras 40%

Special notes

When selecting the *Isosorbide dinitrate 40%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Isosorbide dinitrate 40%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Isosorbide dinit...	12F08-N04	20891	40	20120801
Fagron	Isosorbide dinit...	13D15-N02	21347	39	20130410
Fagron	Isosorbide dinit...	15I10-B01-328577	23200	40	1709092
Fagron	Isosorbide dinit...	17C29-B01-339447	24057	40	20170517

Validation samples

A total of 280317 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 *Isosorbide dinitrate 40%*. These samples are listed above in the [calibration samples](#) section.
- 74337 spectra from a total of 1619 batches from further 372 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 [†].

- 70 spectra of 2 reference samples from the substance/substance group *Isosorbide dinitrate 40%*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Isosorbide dinitrate 40%	15I10-B01-315217	22762	40
Fagron	Isosorbide dinitrate 40%	15I10-B01-328577	23598	30

- 126822 spectra from a total of 2787 batches from further 781 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.

- 306 spectra from 145 *Apo-Ident* customers from 122 batches from the substance/substance group *Isosorbide dinitrate 40%*.

Supplier	Substance	Batch	Spectra
Fagron	Isosorbide dinitrate 40%	11J17-N05	2
Fagron	Isosorbide dinitrate 40%	11D12-N01	2
Fagron	Isosorbide dinitrate 40%	12C08-N05	2

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Supplier	Substance	Batch	Spectra
Fagron	Isosorbide dinitrate 40%	1309210009	1
Sanacorp	Isosorbide dinitrate 40%	11J17-N05	1
Fagron	Isosorbide dinitrate 40%	11I17-N05	1
Fagron	Isosorbide dinitrate 40%	11/17-N05	1
Fagron	Isosorbide dinitrate 40%	9101205	1
Fagron	Isosorbide dinitrate 40%	10029-N10	1
Anzag	Isosorbide dinitrate 40%	12C08-N05	2
Caelo	Isosorbide dinitrate 40%	11D12-N01	1
Fagron	Isosorbide dinitrate 40%	10D29-N10	1
Fagron	Isosorbide dinitrate 40%	12F08-N04	8
Fagron	Isosorbide dinitrate 40%	P11008	1
Fagron	Isosorbide dinitrate 40%	12K14-N02	6
Fagron	Isosorbide dinitrate 40%	13A07-N13	6
Fagron	Isosorbide dinitrate 40%	2413Q03516	1
Fagron	Isosorbide dinitrate 40%	11117-N05	1
Fiebig 23.05.13 ek: 10,...	Isosorbide dinitrate 40%	12F08-N04	1
Caelo	Isosorbide dinitrate 40%	13D15-N02	3
Fagron	Isosorbide dinitrate 40%	13d15-n02	1
Fagron	Isosorbide dinitrate 40%	13D15-N02	7
Fagron	Isosorbide dinitrate 40%	3413U03516	1
Fagron	Isosorbide dinitrate 40%	13A07-0003	1
Phönix	Isosorbide dinitrate 40%	13A07-N13	1
Fagron	Isosorbide dinitrate 40%	11/17-No5	1
Fagron	Isosorbide dinitrate 40%	9E05-N05	1
Euro OTC	Isosorbide dinitrate 40%		1
Fagron	Isosorbide dinitrate 40%	391311-03516	1
Fagron	Isosorbide dinitrate 40%	13F27-N04	6
Fagron	Isosorbide dinitrate 40%	12K14N02	1
Fagron	Isosorbide dinitrate 40%	13I26-N18	9
Fagron	Isosorbide dinitrate 40%	2114M3516	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-294280	8
Fagron	Isosorbide dinitrate 40%	X12010	1
Caelo	Isosorbide dinitrate 40%	13/26-N18	1
Fagron	Isosorbide dinitrate 40%	3211U-03516	1
Fagron	Isosorbide dinitrate 40%	14D09-B03	7
VDI 28.10.14 10,32 euro	Isosorbide dinitrate 40%		1
Fagron	Isosorbide dinitrate 40%	10C19-N01	1
Sanacorp	Isosorbide dinitrate 40%	14D09-B03-294280	1
ebe a	Isosorbide dinitrate 40%	14D09-B03-294281	1
Fagron	Isosorbide dinitrate 40%	12k14-n02	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-294281	3
Fagron	Isosorbide dinitrate 40%	101652	3
Fagron	Isosorbide dinitrate 40%	14D09-B03294282	1
Fagron	Isosorbide dinitrate 40%	12f08-n04	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-294282Eber	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-29481	1
Caelo	Isosorbide dinitrate 40%	14D09B03294281	1
AHD 09.03.2015	Isosorbide dinitrate 40%	14D09-B03-294281	1
Caelo	Isosorbide dinitrate 40%	14D09-B03-294281	2
Fagron	Isosorbide dinitrate 40%	14D09-B03-294282	3
Caelo	Isosorbide dinitrate 40%	13F27-N04	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-300234	13
Allianz Healthcare 17.0...	Isosorbide dinitrate 40%	14D09-B03-300234	1
Fagron	Isosorbide dinitrate 40%	testxx	1
Fagron	Isosorbide dinitrate 40%	14-D09-B03-300234	1
Fagron	Isosorbide dinitrate 40%	4314U-03516	1
Fagron	Isosorbide dinitrate 40%	11F28-N05	2
Caelo	Isosorbide dinitrate 40%	14D09-B03-307018	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-308419	11
Caelo	Isosorbide dinitrate 40%	14D-09-B03-300234	1

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Supplier	Substance	Batch	Spectra
Fagron	Isosorbide dinitrate 40%	14D09-B03-307018	1
Fagron	Isosorbide dinitrate 40%	8564340	1
Caelo	Isosorbide dinitrate 40%	14D09-B03-308419	3
Fagron	Isosorbide dinitrate 40%	14D09-B3-308419	1
Caelo	Isosorbide dinitrate 40%	11/17-N05	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-313566	2
Fagron	Isosorbide dinitrate 40%	14d09-b03-313566	1
Fagron	Isosorbide dinitrate 40%	1216M-03516	1
Fagron	Isosorbide dinitrate 40%	7013190003	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-315217	4
Wepa	Isosorbide dinitrate 40%	14D09-B03-313566	1
Fagron	Isosorbide dinitrate 40%	14D09-B03308419	1
Anzag	Isosorbide dinitrate 40%	1510B01315217	1
Fagron	Isosorbide dinitrate 40%		2
Fargon	Isosorbide dinitrate 40%	15/10-B01-320081	1
Fagron	Isosorbide dinitrate 40%	15I10-B01-315217	2
Noweda	Isosorbide dinitrate 40%	15/10-B01-315217	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-320081	4
Fagron	Isosorbide dinitrate 40%	3115M-03516	1
Fagron	Isosorbide dinitrate 40%	15-10-b01-318522	1
Fagron	Isosorbide dinitrate 40%	160629I	1
Caelo	Isosorbide dinitrate 40%	15/10-B01-320081	4
Fagron	Isosorbide dinitrate 40%	1510B01320081	1
Fagron	Isosorbide dinitrate 40%	15I10-B01	7
Fagron	Isosorbide dinitrate 40%	149168	6
Fagron	Isosorbide dinitrate 40%	15I10-B01-310081	1
Caelo	Isosorbide dinitrate 40%	1510b1320782	1
Fagron	Isosorbide dinitrate 40%	13F27-N040234/1300	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-325474	1
Fagron	Isosorbide dinitrate 40%	1510-b01-325475	3
Fagron	Isosorbide dinitrate 40%	15I10-B01-320782	1
Fagron	Isosorbide dinitrate 40%	15110-B01-320081	1
Fagron	Isosorbide dinitrate 40%	15I10-B01-325474	4
Fagron	Isosorbide dinitrate 40%	1510-B01-320081	1
Fagron	Isosorbide dinitrate 40%	15110-B01-325474	1
Fagron	Isosorbide dinitrate 40%	517I-03516	1
Caelo	Isosorbide dinitrate 40%	15I10-B01	1
Fagron	Isosorbide dinitrate 40%	15-10-b01-325475	1
Fagron	Isosorbide dinitrate 40%	15I10-B01-320081	2
Caelo	Isosorbide dinitrate 40%	1510-B01-315217	1
Fagron	Isosorbide dinitrate 40%	25021711	1
Euro OTC	Isosorbide dinitrate 40%	15I10-B01325474	1
Caelo	Isosorbide dinitrate 40%	15-10b01-328132	1
Fagron	Isosorbide dinitrate 40%	1510-B01320081	1
Fagron	Isosorbide dinitrate 40%	1510-b01-328132	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-325474	2
Fagron	Isosorbide dinitrate 40%	151-b01-328132	2
Fagron	Isosorbide dinitrate 40%	15I10-B01-328132	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-328577	1
Fagron	Isosorbide dinitrate 40%	15/10-b01-331287	3
Fagron	Isosorbide dinitrate 40%	15/10-B01-328132	2
Ebert-Jacobi	Isosorbide dinitrate 40%	15I10-B01-328132	1
Anzag	Isosorbide dinitrate 40%	15/10-B01-328577	1
Fagron	Isosorbide dinitrate 40%	15I10-B01-328577	2
Fagron	Isosorbide dinitrate 40%	15/10-b01-328132	3
Fagron	Isosorbide dinitrate 40%	1510B01328577	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-331287	1
Fagron	Isosorbide dinitrate 40%	15-10-b01-331287	5
Fagron	Isosorbide dinitrate 40%	17c29-b01-335071	6
Frago/Gehe	Isosorbide dinitrate 40%	17C29-B01-335070	1

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Supplier	Substance	Batch	Spectra
Fagron	Isosorbide dinitrate 40%	17C29-B01-335070	7
Frago/Noweda	Isosorbide dinitrate 40%	15I10-B01-328577	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-335071	1
Frago/Noweda	Isosorbide dinitrate 40%	17C29-B01-335070	1
Ichthyol-Gesellschaft	Isosorbide dinitrate 40%	17C29-B01-335070	1
Caelo	Isosorbide dinitrate 40%	15-10-b01-328132	2
Fargon/Gehe	Isosorbide dinitrate 40%	17C29-B01-339447	1
Fagron	Isosorbide dinitrate 40%	17c29-b01-339448	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-339448	1
Fagron	Isosorbide dinitrate 40%	17C29-b01-339448	1
Fagron	Isosorbide dinitrate 40%	17C29-B01	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-339447	3
Fagron	Isosorbide dinitrate 40%	193469	2
Caelo	Isosorbide dinitrate 40%	17c29-b01-347885	4
Caelo	Isosorbide dinitrate 40%	701319-0003	1
Sanacorp	Isosorbide dinitrate 40%	193469	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-347589	3
GEHE	Isosorbide dinitrate 40%	17C29-B01-347589	1
Fagron	Isosorbide dinitrate 40%	17C29-801-347885	1
Fagron	Isosorbide dinitrate 40%	17C-B01-347589	1
Caelo	Isosorbide dinitrate 40%	17C29-B01-339447	1
Caelo	Isosorbide dinitrate 40%	17C29-B01-348859	1
Fagron	Isosorbide dinitrate 40%	17C29B01339447	1
Fagron	Isosorbide dinitrate 40%	17C29B01347589	1
Caelo	Isosorbide dinitrate 40%	193469	1
Fagron	Isosorbide dinitrate 40%	17C29B01348859	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-348859	4
Fagron	Isosorbide dinitrate 40%	17C29-B01-350469	3
Fagron	Isosorbide dinitrate 40%	17C29-B01350469	1
	Isosorbide dinitrate 40%	17c29-b01-348859	1

- 78 623 spectra from 565 *Apo-Ident* customers from a total of 26 015 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Isosorbide dinitrate 40%* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Isosorbide dinitrate 40%* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 337
Type B	0	70	0	126 822
Type C	0	302	4	78 623

The substance/substance group *Isosorbide dinitrate 40%* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2264 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 91.4286 %)
Type C	100.0000 % (> 99.8817 %)	98.6928 % (> 97.7124 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20891	23200	8.34	41.68
21347	23200	5.35	41.65
23200	23200	0.00	42.24
24057	23200	8.39	42.40

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Isoxuprine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22640-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Isoxuprine hydrochloride; Isoxsuprini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Isoxuprine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Isoxuprine hydro...	161770	22640	40	20160818*
Euro OTC	Isoxuprine hydro...	1503008-01	22659	40	20150430
Caelo	Isoxuprine hydro...	181078	24252	40	20180719*

Validation samples

A total of 280 317 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 *Isoxuprine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Isoxuprine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Isoxuprine hydrochloride	16177001	22735	40

- 126 852 spectra from a total of 2788 batches from further 781 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 *Isoxuprine hydrochloride*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

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

Validation results

The validation runs checked whether the substance/substance group *Isoxuprine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Isoxuprine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	40	0	126 852
Type C	0	0	0	78 929

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
22640	22640	0.00	48.57
22659	22640	1.93	48.57
24252	24252	0.00	48.86

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ketamine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20278-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ketamine hydrochloride; Ketamini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ketamine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ketamine hydroch...	13H19-N01	21044	40	8931
Fagron	Ketamine hydroch...	14I03-B02-303165	21779	40	20140926
Fagron	Ketamine hydroch...	14I03-B02-311706	22533	40	20140926

Validation samples

A total of 280 317 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 *Ketamine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Ketamine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ketamine hydrochloride	14I03-B02-303165	21779 [†]	20
Fagron	Ketamine hydrochloride	15E07-B03-322164	23201	40
Fagron	Ketamine hydrochloride	16E18-B03-339897	23941	40

- 126 792 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 18 spectra from 10 *Apo-Ident* customers from 14 batches from the substance/substance group *Ketamine hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	Ketamine hydrochloride	182513P	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
Fagron	Ketamine hydrochloride	14/03-B02-303165	1
GEHE 27.05.2014	Ketamine hydrochloride	13H19-N01	1
Fagron	Ketamine hydrochloride	14I03-B02-309852	1
Noweda	Ketamine hydrochloride	14/03-B02-311706	1
Noweda	Ketamine hydrochloride	292414P	1
phönix	Ketamine hydrochloride	14I03-B02-311706	1
Fagron	Ketamine hydrochloride	15E07-B03-322164	5
Fagron	Ketamine hydrochloride	16E18-B03-328264	1
Fagron	Ketamine hydrochloride	16E18-B03-332957	1
Fagron	Ketamine hydrochloride	16E18-B03-334370	1
Fagron	Ketamine hydrochloride	16E18-B03	1
Fagron	Ketamine hydrochloride	16E18-B03-339897	1
Fagron	Ketamine hydrochloride	17K14-B01-347995	1

- 78 911 spectra from 565 *Apo-Ident* customers from a total of 26 123 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ketamine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ketamine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	11	7	78 911

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
21044	21044	0.00	67.78
21779	21044	5.13	69.01
22533	21044	4.27	68.49

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ketoconazole**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20688-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ketoconazole; Ketoconazolum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Ketoconazole*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ketoconazole	12171007	20688	30	1401554
Fagron	Ketoconazole	12A16-N06	20699	40	20120123
Caelo	Ketoconazole	13179612	21514	40	20130613
Caelo	Ketoconazole	13179612	21515	40	20130613

Validation samples

A total of 280317 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 *Ketoconazole*. These samples are listed above in the [calibration samples](#) section.
- 74346 spectra from a total of 1620 batches from further 372 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 *Ketoconazole*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ketoconazole	13179612	21514 [†]	20
Caelo	Ketoconazole	13179612	21515 [†]	20
Fagron	Ketoconazole	16A26-B01-322982	23183	40
Fagron	Ketoconazole	17H14-B01-339422	23917	40
Caelo	Ketoconazole	153477	24028	40

- 126732 spectra from a total of 2785 batches from further 781 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.

- 80 spectra from 41 *Apo-Ident* customers from 40 batches from the substance/substance group *Ketoconazole*.

[†]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
Gehe	Ketoconazole	11070019	1
Caelo	Ketoconazole	11070001	1
Caelo	Ketoconazole	12300406	1
Caelo	Ketoconazole	11070022	1
Phönix	Ketoconazole	12171018	1
Fagron	Ketoconazole	12I17-N02	1
Phönix	Ketoconazole	13179602	3
Caelo	Ketoconazole	53317046	2
Caelo	Ketoconazole	12300407	2
Caelo	Ketoconazole	13179601	1
Caelo	Ketoconazole	13179606	3
Caelo	Ketoconazole	13179612	2
Fagron	Ketoconazole	13H09-N07	1
Fagron	Ketoconazole	13J23-N04	1
ANZAG 23.07.14	Ketoconazole	13h09-n07	1
Caelo	Ketoconazole	13399404	8
Fagron	Ketoconazole	13179613	1
Caelo	Ketoconazole	13399408	6
Fagron	Ketoconazole	14E09-B01-293736	3
Fagron	Ketoconazole	14E09-B01-297637	2
Caelo	Ketoconazole	13399412	1
Fagron	Ketoconazole	14K04-B06-309671	2
Fagron	Ketoconazole	5015E-02866	1
Caelo	Ketoconazole	14350408	1
Caeolo /Gehe	Ketoconazole	14350408	1
Caelo	Ketoconazole	14350416	3
Fagron	Ketoconazole	15G23-B03-312063	1
Caelo	Ketoconazole	14350421	1
Caelo	Ketoconazole	14350422	3
Caelo	Ketoconazole	14350427	2
Caelo	Ketoconazole	14350429	3
Caelo	Ketoconazole	14350436	2
Caelo	Ketoconazole	14350419	1
Fagron	Ketoconazole	15G23-B03-316596	1
Caelo	Ketoconazole	14350420	2
Fagron	Ketoconazole	16A26-B01-327490	1
Caelo	Ketoconazole	14350437	4
Caelo	Ketoconazole	14350442	3
Fagron	Ketoconazole	16A26-B01-335467	1
Caelo	Ketoconazole	15347701	2
Caelo	Ketoconazole	18007003	2

- 78 849 spectra from 565 *Apo-Ident* customers from a total of 26 097 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ketoconazole* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ketoconazole* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 346
Type B	0	160	0	126 732
Type C	0	77	3	78 849

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	96.2500 % (> 92.5000 %)

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
20688	20688	0.00	74.25
20699	20688	15.68	76.26
21514	20688	16.76	76.31
21515	20688	17.64	76.68

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Lactose monohydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20029-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lactose monohydrate; Lactosum monohydricum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Lactose monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lactose monohydr...	12139910	20685	30	20120606
Caelo	Lactose monohydr...	14025601	21525	40	20140207
Euro OTC	Lactose monohydr...	1509030	21935	40	20151013*
Caelo	Lactose monohydr...	160277	22460	40	20160321*
Euro OTC	Lactose monohydr...	1606025	22701	40	20160628*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 190 spectra of 5 reference samples from the substance/substance group *Lactose monohydrate*. These samples are listed above in the [calibration samples](#) section.
- 74306 spectra from a total of 1618 batches from further 372 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 [†].

- 400 spectra of 11 reference samples from the substance/substance group *Lactose monohydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lactose monohydrate	14025601	21526	40
Caelo	Lactose monohydrate	14025601	21527	40
Caelo	Lactose monohydrate	14025601	21528	40
Caelo	Lactose monohydrate	14025601	21529	40
Euro OTC	Lactose monohydrate	1509030	21935 [†]	20
Caelo	Lactose monohydrate	160277	22460 [†]	20
Caelo	Lactose monohydrate	15236220	22584	40
Euro OTC	Lactose monohydrate	1703019	23141	40
Caelo	Lactose monohydrate	173360	23828	40
Euro OTC	Lactose monohydrate	1802002	23962	40
Euro OTC	Lactose monohydrate	1812008	24415	40

- 126492 spectra from a total of 2781 batches from further 781 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.

- 951 spectra from 229 *Apo-Ident* customers from 360 batches from the substance/substance group *Lactose monohydrate*.

Supplier	Substance	Batch	Spectra
Caelo	Lactose monohydrate	11219208	3
Caelo	Lactose monohydrate	11079002	2
Spangropharm	Lactose monohydrate	91444379	1
Fagron	Lactose monohydrate	11L22-N03	1
Caelo	Lactose monohydrate	12021502	1
Bahnhof-Apotheke	Lactose monohydrate	120614	1
EuRho	Lactose monohydrate	1112020-01	1
Caelo	Lactose monohydrate	3788916	2
Caelo	Lactose monohydrate	12021508	1
Caelo	Lactose monohydrate	12021518	5
Fagron	Lactose monohydrate	12G27-N02	5
Euro OTC	Lactose monohydrate	1112020-01	2
Bahnhof-Apotheke	Lactose monohydrate	120808	1
Caelo	Lactose monohydrate		1
Caelo	Lactose monohydrate	30101201	1
vdl	Lactose monohydrate	1112020-01	2
Caelo	Lactose monohydrate	12139908	1
Caelo	Lactose monohydrate	12139901	2
Caelo	Lactose monohydrate	12139914	6
Fagron	Lactose monohydrate	12C26-N05	1
Anzag 29.11.12 ek:7,51	Lactose monohydrate	12139914	1
Gehe	Lactose monohydrate	1112020-01	1
Caelo	Lactose monohydrate	1106022-02	1
Bahnhof-Apotheke	Lactose monohydrate	121119	2
Fagron	Lactose monohydrate	11C29-N06	1
Eigenherstellung	Lactose monohydrate	40113HJK01	1
Anzag	Lactose monohydrate	12139915	5
Eigenherstellung	Lactose monohydrate	70113HML01	1
Caelo	Lactose monohydrate	17011302	1
Caelo	Lactose monohydrate	2901312210	1
Euro OTC	Lactose monohydrate	1112020-02	4
Caelo	Lactose monohydrate	11014714	1
Gehe	Lactose monohydrate	1112020-02	3
Caelo	Lactose monohydrate	12139915	3
Caelo	Lactose monohydrate	12139920	6
Caelo	Lactose monohydrate	1301C005	2
Caelo	Lactose monohydrate	11219216	1
Bahnhof-Apotheke	Lactose monohydrate	130115	1
Caelo	Lactose monohydrate	12336801	7
Caelo	Lactose monohydrate	12139910	1
Fagron	Lactose monohydrate	1301C007-278131	1
A.H.D.	Lactose monohydrate	12336801	1
Caelo	Lactose monohydrate	12139912	1
Caelo	Lactose monohydrate	12139909	1
Euro OTC	Lactose monohydrate	110602202	1
Europarm/Otto	Lactose monohydrate	1106022-01	1
Caelo	Lactose monohydrate	12336815	9
Fagron	Lactose monohydrate	1303C003-280390	1
Bombastus	Lactose monohydrate	275194/0	1
Bombastus	Lactose monohydrate	272680/0	1
Bombastus	Lactose monohydrate	275225/0	1
Euro OTC	Lactose monohydrate	1301028-01	8

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Supplier	Substance	Batch	Spectra
Caelo	Lactose monohydrate	12336816	2
Fagron	Lactose monohydrate	1301C006-278128	6
Bombastus	Lactose monohydrate	274926	1
Noweda/ Caesar&Loretz	Lactose monohydrate	12336815	1
Alliance Healthcare	Lactose monohydrate	10195101	2
Caelo	Lactose monohydrate	s-100513-1	1
Caelo	Lactose monohydrate	12336820	2
Caelo	Lactose monohydrate	1071302	1
Sanacorp	Lactose monohydrate	12336815	1
Caelo	Lactose monohydrate	13104902	7
Anzag / Noweda	Lactose monohydrate	12336815	1
Fagron	Lactose monohydrate	12C09-N04	1
Caelo	Lactose monohydrate	12336814	1
Cealo	Lactose monohydrate	13104901	1
Caelo	Lactose monohydrate	10195107	2
Fagron	Lactose monohydrate	1303C003	1
Phönix	Lactose monohydrate	12336815	1
Euro OTC	Lactose monohydrate	130102801	1
Caelo	Lactose monohydrate	13081302	1
Caelo	Lactose monohydrate	13104901	5
Fagron	Lactose monohydrate	1301C005-278129	2
Sanacorp	Lactose monohydrate	13104901	1
cesar&lorentz/Phönix	Lactose monohydrate	12336815	1
Caelo	Lactose monohydrate	6091301	1
Bahnhof-Apotheke	Lactose monohydrate	130729	1
EuRho	Lactose monohydrate	1301028-01	1
Fagron	Lactose monohydrate	1303C001	1
Eigenherstellung	Lactose monohydrate	110913HJK01	1
Caelo	Lactose monohydrate	160913PJK01	1
Caelo	Lactose monohydrate	13104908	2
Fagron	Lactose monohydrate	1303C002-280398	1
Euro OTC	Lactose monohydrate	1301028-02	12
Bahnhof-Apotheke	Lactose monohydrate	130911	1
Bahnhof-Apotheke	Lactose monohydrate	130925	1
Caelo	Lactose monohydrate	4313Q2210	1
Caesar /phönix	Lactose monohydrate	13104901	2
Europ Ots Pharma	Lactose monohydrate	1301028-02	3
Caelo	Lactose monohydrate	13104909	5
Euro OTC	Lactose monohydrate	31102013A	1
Caelo	Lactose monohydrate	13104909-3422310182	1
Sanacorp	Lactose monohydrate	13104909	1
Fagron	Lactose monohydrate	13E23-B01-283334	1
Bahnhof-Apotheke	Lactose monohydrate	131023	1
Caelo	Lactose monohydrate	13104911	2
Gehe	Lactose monohydrate	1301028-02	2
Caelo	Lactose monohydrate	13104910	2
schubert / Phoenix	Lactose monohydrate	1334PLV-1775	1
Bahnhof-Apotheke	Lactose monohydrate	131112	1
Caelo	Lactose monohydrate	13104909-3453311172	1
Caelo	Lactose monohydrate	13104912	1
Fagron	Lactose monohydrate	13E23-B01	2
Caelo	Lactose monohydrate	13299101	9
Bombastus	Lactose monohydrate	283992	2
Bombastus	Lactose monohydrate	282648	1
Bahnhof-Apotheke	Lactose monohydrate	131127	2
Caelo	Lactose monohydrate	13299102	12
Fragon	Lactose monohydrate	10706040	1
Peter Kölln	Lactose monohydrate	229719241-0640	1
Bahnhof-Apotheke	Lactose monohydrate	131218	2
Caelo	Lactose monohydrate	24011405	1

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Supplier	Substance	Batch	Spectra
Bahnhof-Apotheke	Lactose monohydrate	140113	3
Phönix	Lactose monohydrate	13299102	2
Caelo	Lactose monohydrate	8021401	1
Fagron	Lactose monohydrate	1303C001-280388	1
Fagron	Lactose monohydrate	13E23-B01-283332	2
Caelo	Lactose monohydrate	20021411	1
Caelo	Lactose monohydrate	13299107	5
Bahnhof-Apotheke	Lactose monohydrate	140206	2
Sanacorp	Lactose monohydrate	13299102	1
Caelo	Lactose monohydrate	7031402	1
Caelo	Lactose monohydrate	13299108	5
Caelo	Lactose monohydrate	12399107	1
Caelo	Lactose monohydrate	13299103	1
Bombastus	Lactose monohydrate	282696/0	1
Fagron	Lactose monohydrate	282567/0	1
Bombastus	Lactose monohydrate	284321/0	1
Bahnhof-Apotheke	Lactose monohydrate	140310	2
Fagron	Lactose monohydrate	13I23-B03	4
Euro OTC	Lactose monohydrate	L1237A4172	2
Euro OTC	Lactose monohydrate	1401003-01	9
Phoenix 19.03.2014	Lactose monohydrate	13104909	1
Bahnhof-Apotheke	Lactose monohydrate	140220	1
Caelo	Lactose monohydrate	12041401	1
Fagron	Lactose monohydrate	12/23-B02-287554	1
Fagron	Lactose monohydrate	13/23-B02-287554	1
Bahnhofsapotheke	Lactose monohydrate	140401	1
Caelo	Lactose monohydrate	14025608	2
Caelo	Lactose monohydrate	9051401	1
Caelo	Lactose monohydrate	14025603	7
Caelo	Lactose monohydrate	14025601	3
Caelo	Lactose monohydrate	14025604	6
Bombastus	Lactose monohydrate	286697/0	1
Bombastus	Lactose monohydrate	288015/0	1
Bombastus	Lactose monohydrate	285087/0	1
	Lactose monohydrate	14025604	1
Caelo	Lactose monohydrate	140612	3
Sanacorp	Lactose monohydrate	13299108	1
Gatt-Koller / Phoenix	Lactose monohydrate	5580/12120813	2
GEHE am 17.06.2014	Lactose monohydrate	13299108	1
Noweda	Lactose monohydrate	14025601	1
Euro OTC	Lactose monohydrate	140-1003-01	1
Caelo	Lactose monohydrate	1401003-01	1
Caelo	Lactose monohydrate	26071401	1
Phoenix	Lactose monohydrate	1404PLV-1928	4
Eigenherstellung	Lactose monohydrate	60814HSA01	1
Bahnhof-Apotheke	Lactose monohydrate	140630	1
Euro OTC	Lactose monohydrate	18082014A	1
Caelo	Lactose monohydrate	14025616	3
Caelo	Lactose monohydrate	3091405	1
Fagron	Lactose monohydrate	13I23-B03-291116	1
Euro OCT	Lactose monohydrate	1401003-01	3
Euro OTC	Lactose monohydrate	14025604	2
Caelo	Lactose monohydrate	14140304	2
Caelo	Lactose monohydrate	14140302	4
Bombastus	Lactose monohydrate	288927	1
Bombastus	Lactose monohydrate	289238	1
Caelo	Lactose monohydrate	1402504	1
Fagron	Lactose monohydrate	13I23-B03-291115	1
Caelo	Lactose monohydrate	14025620	11
Bombastus	Lactose monohydrate	13299108	1

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Supplier	Substance	Batch	Spectra
Fagron	Lactose monohydrate	10726158	1
Euro OTC	Lactose monohydrate	5123	1
Caelo	Lactose monohydrate	23101404	1
Fagron	Lactose monohydrate	13I23-B03-287414	1
AHD	Lactose monohydrate	13I23-B03-291114	1
Caelo	Lactose monohydrate	14140305	6
Phönix	Lactose monohydrate	14025616	1
Caelo	Lactose monohydrate	7111402	1
Euro OTC	Lactose monohydrate	14025616	2
otz pharma	Lactose monohydrate	130102802	1
Fagron	Lactose monohydrate	13J23-B03-291114	1
Caelo	Lactose monohydrate	3121406	1
Caelo	Lactose monohydrate	14140308	6
Caelo	Lactose monohydrate	14025619	3
Fagron	Lactose monohydrate	14A30-B07	2
Caelo	Lactose monohydrate	14140309	2
Fagron	Lactose monohydrate	14A30-B07-296182	2
Euro OTC	Lactose monohydrate	1401003-02	5
Bombastus	Lactose monohydrate	291464	1
Caelo	Lactose monohydrate	3031501	1
Caelo	Lactose monohydrate	14333503	1
Fagron	Lactose monohydrate	14140312	1
Sanacorp	Lactose monohydrate	14025620	1
Caelo	Lactose monohydrate	14333502	2
Caelo	Lactose monohydrate	30031503	1
Caelo	Lactose monohydrate	14140312	13
Nachprüfung	Lactose monohydrate	3712Q-02210	1
Caelo	Lactose monohydrate	200415HJK02	1
Euroo/Phoenix	Lactose monohydrate	1401003-02	1
Caelo	Lactose monohydrate	14333508	1
Caelo	Lactose monohydrate	14333501	3
Caelo	Lactose monohydrate	14333511	5
Caelo	Lactose monohydrate	14333510	1
Fagron	Lactose monohydrate	14H27-B02	1
Caelo	Lactose monohydrate	23051501	1
Caesar u. Loretz	Lactose monohydrate	14025620	1
Caelo	Lactose monohydrate	14333509	10
Fagron	Lactose monohydrate	15A19-B06-303437	3
Caelo	Lactose monohydrate	1501017-01	4
Caelo	Lactose monohydrate	5061504	1
Caelo	Lactose monohydrate	1433502	1
Caelo	Lactose monohydrate	14333513	5
Fagron	Lactose monohydrate	14H27-B01-305666	1
Caelo	Lactose monohydrate	1433510	1
Caelo	Lactose monohydrate	23061504	1
Fagron	Lactose monohydrate	10751120	1
Caelo	Lactose monohydrate	8071501	1
Fagron	Lactose monohydrate	15A19-B06	3
Europ Ots Pharma	Lactose monohydrate	1401003-02	1
Euro OTC	Lactose monohydrate	1013Q-02210	1
Caelo	Lactose monohydrate	14333518	3
Sanacorp	Lactose monohydrate	14333509	1
Sanacorp	Lactose monohydrate	14333518	1
Eigenherstellung	Lactose monohydrate	40815HMS01	1
Caelo	Lactose monohydrate	143335114	1
Caelo	Lactose monohydrate	14333521	7
Fagron	Lactose monohydrate	14333518	1
Fagron	Lactose monohydrate	14333525	1
Euro OTC	Lactose monohydrate	1501017-01	10
Bombastus	Lactose monohydrate	294897/0	1

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Supplier	Substance	Batch	Spectra
Caelo	Lactose monohydrate	14333520	8
Bombastus	Lactose monohydrate	295011/0	1
Bombastus	Lactose monohydrate	294184/0	1
Bombastus	Lactose monohydrate	293918/0	1
Caelo	Lactose monohydrate	14333514	1
Caelo	Lactose monohydrate	1433521	1
Caelo	Lactose monohydrate	15236204	8
Anzag/Fragon	Lactose monohydrate	1005SLP	1
Caelo	Lactose monohydrate	15236201	18
Caelo	Lactose monohydrate	14333528	2
Caelo	Lactose monohydrate	1433518	2
Caelo	Lactose monohydrate	15011701	1
Euro OTC	Lactose monohydrate	1501017-02	1
Euro OTC	Lactose monohydrate	1401003	1
Caelo	Lactose monohydrate	15236208	11
Euro OTC	Lactose monohydrate	1509030-01	6
Caelo/Noweda	Lactose monohydrate	1523204	1
Caelo	Lactose monohydrate	15236214	6
Rondell Apotheke	Lactose monohydrate	1509030-01	2
Caelo	Lactose monohydrate	15236203	2
Caelo	Lactose monohydrate	1090216	1
Caelo	Lactose monohydrate	1526201	1
Caelo	Lactose monohydrate	15236209	7
EuRho	Lactose monohydrate	1501017-01	1
Euro OTC	Lactose monohydrate	15010	1
Fagron	Lactose monohydrate	15A19-B06-303439	3
Fagron	Lactose monohydrate	14H27-B02-302033	1
Caelo	Lactose monohydrate	15236213	2
Caelo	Lactose monohydrate	1433520	1
Caelo	Lactose monohydrate	15236217	1
Phoenix	Lactose monohydrate	15A19-B06	3
Fagron	Lactose monohydrate	15H14-B03-314451	3
Caelo	Lactose monohydrate	15236215	3
Caesar & Loretz/Noweda	Lactose monohydrate	15236204	1
Euro OTC	Lactose monohydrate	3215A-02210	1
Caelo	Lactose monohydrate	15236202	1
pharmachem	Lactose monohydrate	15236208	1
Euro OTC	Lactose monohydrate	1301028-03	2
Caelo	Lactose monohydrate	15236221	4
Caelo	Lactose monohydrate	16027703	6
Ebert u. Jacobi 18.0...	Lactose monohydrate	15236215	1
Caelo	Lactose monohydrate	15236220	3
Caelo	Lactose monohydrate	16027702	6
Caelo	Lactose monohydrate	152362	2
Euro OTC	Lactose monohydrate	1509030-02	5
Caelo	Lactose monohydrate	16027706	5
Caelo	Lactose monohydrate	16027707	2
Caelo	Lactose monohydrate	1509030-02	1
Caelo	Lactose monohydrate	16027704	1
Caelo	Lactose monohydrate	150903002	1
Euro OTC	Lactose monohydrate	150101701	1
Caesar u Loretz	Lactose monohydrate	1433520	1
Caelo	Lactose monohydrate	16027701	3
Caelo	Lactose monohydrate	123test	1
Euro OTC	Lactose monohydrate	15090-30-02	1
Caelo	Lactose monohydrate	123Test	1
Euro OTC	Lactose monohydrate	1606025-01	21
Caelo	Lactose monohydrate	16027708	6
Caesar & Loretz GmbH	Lactose monohydrate	14140311	1
Euro OTC	Lactose monohydrate	150903002	1

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Supplier	Substance	Batch	Spectra
Edelweiss	Lactose monohydrate	253292176-1124	1
Alte Apotheke	Lactose monohydrate	16027708	1
Bombastus	Lactose monohydrate	306147	3
Bombastus	Lactose monohydrate	305227	2
Bombastus	Lactose monohydrate	293289	1
Bombastus	Lactose monohydrate	3020165	1
Bombastus	Lactose monohydrate	300657	2
Bombastus	Lactose monohydrate	304755	1
Bombastus	Lactose monohydrate	303658	2
Bombastus	Lactose monohydrate	2932880	1
Bombastus	Lactose monohydrate	295476	1
Bombastus	Lactose monohydrate	293649	1
Bombastus	Lactose monohydrate	295714	1
Bombastus	Lactose monohydrate	293074	1
Bombastus	Lactose monohydrate	293970	1
Bombastus	Lactose monohydrate	292996	1
Bombastus	Lactose monohydrate	292995	1
Bombastus	Lactose monohydrate	286710	1
Bombastus	Lactose monohydrate	286354	1
Bombastus	Lactose monohydrate	292983	1
Bombastus	Lactose monohydrate	294154	1
Bombastus	Lactose monohydrate	293290	1
EuRho	Lactose monohydrate	1509030-02	1
Caelo	Lactose monohydrate	16231203	4
Caelo	Lactose monohydrate	16231202	10
Bombastus	Lactose monohydrate	292982	2
Bombastus	Lactose monohydrate	305336	2
Bombastus	Lactose monohydrate	306850	1
Bombastus	Lactose monohydrate	306652	1
Bombastus	Lactose monohydrate	306964	1
Bombastus	Lactose monohydrate	306990	1
Chiesi	Lactose monohydrate	16027708	1
Caelo	Lactose monohydrate	16231201	3
Bombastus	Lactose monohydrate	306651/0	1
Bombastus	Lactose monohydrate	305227/0	1
Bombastus	Lactose monohydrate	305336/0	1
siehe Protokoll	Lactose monohydrate	1606025-01	1
Caelo	Lactose monohydrate	16231207	7
Caesar u Loretz	Lactose monohydrate	16231202	1
Bombastus	Lactose monohydrate	307573/0	1
Caelo	Lactose monohydrate	123456	1
Caelo	Lactose monohydrate	16231208	5
Bombastus	Lactose monohydrate	307543	2
Bombastus	Lactose monohydrate	306989	2
Bombastus	Lactose monohydrate	307741	1
Caelo	Lactose monohydrate	5041702	1
Bombastus	Lactose monohydrate	3077410	1
Caelo	Lactose monohydrate	16231211	13
Caelo	Lactose monohydrate	16231206	4
Sanacorp,05.04.17, 5,96EUR	Lactose monohydrate	16231202	1
Caelo	Lactose monohydrate	16321202	1
Caelo	Lactose monohydrate	1623120803815470	1
Bombastus	Lactose monohydrate	308118/0	1
Bombastus	Lactose monohydrate	307702/0	1
Bombastus	Lactose monohydrate	307976/0	1
Bombastus	Lactose monohydrate	307444/0	1
phönix	Lactose monohydrate	16231202	1
Caelo	Lactose monohydrate	2051702	1
Caelo	Lactose monohydrate	16231214	5
Caelo	Lactose monohydrate	16231202	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Lactose monohydrate	160602501	1
Euro OTC	Lactose monohydrate	1606025-02	2
Caelo	Lactose monohydrate	10071701	1
Bombastus	Lactose monohydrate	309508	1
Bombastus	Lactose monohydrate	308438	1
Bombastus	Lactose monohydrate	309351	1
Caelo	Lactose monohydrate	16231212	5
Gehe	Lactose monohydrate	16231211	1
Caelo	Lactose monohydrate	16231213	1
Bombastus	Lactose monohydrate	309413/0	1
	Lactose monohydrate	309351/0	1
Bombastus	Lactose monohydrate	308117	1
	Lactose monohydrate	309508/0	1
Bombastus	Lactose monohydrate	309509	1
Finteler Apotheke	Lactose monohydrate	16231211	1
Caelo	Lactose monohydrate	15081701	1
Caelo	Lactose monohydrate	16091710	1
Caelo	Lactose monohydrate	1703019-01	3
Caelo	Lactose monohydrate	6101702	1
gehe	Lactose monohydrate	16231211	1
Caelo	Lactose monohydrate	17078307	4
Caelo	Lactose monohydrate	17078306	6
Caelo	Lactose monohydrate	27101702	1
Bombastus	Lactose monohydrate	311280/0	1
Bombastus	Lactose monohydrate	308117/0	1
Bombastus	Lactose monohydrate	311362/0	1
Bombastus	Lactose monohydrate	310691/0	1
Bombastus	Lactose monohydrate	310912/0	1
Bombastus	Lactose monohydrate	309509/0	1
Bombastus	Lactose monohydrate	310082/0	1
Bombastus	Lactose monohydrate	310905/0	1
Caelo	Lactose monohydrate	16231215	1
Bombastus	Lactose monohydrate	311280	1
Bombastus	Lactose monohydrate	17000754	1
Bombastus	Lactose monohydrate	310691	1
Bombastus	Lactose monohydrate	310905	1
Bombastus	Lactose monohydrate	17001199	1
Bombastus	Lactose monohydrate	17001212	1
Fagron	Lactose monohydrate	16231215	1
Noweda	Lactose monohydrate	1703019-01	1
Caelo	Lactose monohydrate	17078303	14
Sanacorp	Lactose monohydrate	17078303	1
Fagron	Lactose monohydrate	1623123	1
Fagron	Lactose monohydrate	17078302	1
Caelo	Lactose monohydrate	17078312	9
Euro OTC	Lactose monohydrate	1703019-01	2
Noweda	Lactose monohydrate	16231215	1
Noweda	Lactose monohydrate	17078303	1
Caelo	Lactose monohydrate	162312135465	1
Caelo	Lactose monohydrate	17078302	2
Caelo	Lactose monohydrate	1703019-020	1
Euro OTC	Lactose monohydrate	UP250171017	1
Caelo	Lactose monohydrate	17321001	10
Caelo	Lactose monohydrate	17321004	3
EuRho	Lactose monohydrate	170301901	3
Sanacorp	Lactose monohydrate	17321004	1
Kehr	Lactose monohydrate	17321004	1
Euro OTC	Lactose monohydrate	1703019-02	3
GEHE	Lactose monohydrate	17321001	1
Fagron	Lactose monohydrate	17321001	1

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Supplier	Substance	Batch	Spectra
Caelo	Lactose monohydrate	11041801	1
Caelo	Lactose monohydrate	17321005	1
Caelo	Lactose monohydrate	17321002	3
Caelo	Lactose monohydrate	9061803	1
Caelo	Lactose monohydrate	17078303-20180619Ma2	1
Caelo	Lactose monohydrate	26061801	1
Caelo	Lactose monohydrate	17336005	4
Caelo	Lactose monohydrate	17336001	1
Caelo	Lactose monohydrate	21071801	1
Caelo	Lactose monohydrate	17336009	4
Caelo	Lactose monohydrate	17336007	13
Caelo	Lactose monohydrate	30081801	1
Caelo	Lactose monohydrate	17336008	4
Euro OTC	Lactose monohydrate	180200201	1
Euro OTC	Lactose monohydrate	1802002-01	1
Fagron	Lactose monohydrate	1802002-01	1
Caelo	Lactose monohydrate	21111813	1
Caelo	Lactose monohydrate	2011901	1
Caelo	Lactose monohydrate	5011901	1
Caelo	Lactose monohydrate	17336013	2
Caelo	Lactose monohydrate	18198001	1
Caelo	Lactose monohydrate	1802002-01	1

- 77 978 spectra from 565 *Apo-Ident* customers from a total of 25 787 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	190	0	74 306
Type B	0	400	0	126 492
Type C	0	932	19	77 978

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.8421 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.5000 %)
Type C	100.0000 % (> 99.8817 %)	98.0021 % (> 97.6866 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20685	22460	3.21	45.08
21525	22460	6.12	43.15
21935	21935	0.00	47.56
22701	22701	0.00	46.65
22460	22460	0.00	47.35

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Levocarnitine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20357-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Levocarnitine; Levocarnitivum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Levocarnitine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Levocarnitine	1210029-01	20809	40	20121130
Fagron	Levocarnitine	12H10-N07	20818	40	20120830
Fagron	Levocarnitine	14A20-B11-290728	21790	40	AR-15-FG-016322-01
Fagron	Levocarnitine	14A20-B11-290728	21968	40	AR-16-FG-005969-01
Fagron	Levocarnitine	15L04-B05-319229	23194	40	AR-17-FG-012937-01
Fagron	Levocarnitine	16L06-B03-338285	23919	40	20161227

Validation samples

A total of 280317 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 *Levocarnitine*. These samples are listed above in the [calibration samples](#) section.
- 74256 spectra from a total of 1618 batches from further 372 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 *Levocarnitine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Levocarnitine	1303027-02	21648	60
Fagron	Levocarnitine	14A20-B11-290728	21790 [†]	20
Fagron	Levocarnitine	14A20-B11-290728	21968 [†]	20
Fagron	Levocarnitine	16F20-B01-326616	23402	40
Fagron	Levocarnitine	17K23-B01-345633	24009	40

- 126712 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 7 spectra from 6 *Apo-Ident* customers from 6 batches from the substance/substance group *Levocarnitine*.

[†]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
Fagron	Levocarnitine	13G19-N12	2
Euro OTC	Levocarnitine	1303027	1
Fagron	Levocarnitine	13111701	1
Fagron	Levocarnitine	9041504	1
Euro OTC	Levocarnitine	L1608038-01	1
Denk	Levocarnitine	A04217	1

- 78 922 spectra from 565 *Apo-Ident* customers from a total of 26 131 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Levocarnitine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Levocarnitine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	180	0	126 712
Type C	0	7	0	78 922

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8818 %)	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
21968	21968	0.00	65.64
20809	23194	16.16	33.09
20818	23194	21.28	36.03
21790	21790	0.00	58.80
23194	23194	0.00	38.18
23919	23194	9.34	37.57

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Levothyroxin sodium**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21708-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Levothyroxin sodium; Levothyroxinum natrii

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Levothyroxin sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Levothyroxin sod...	14E28-B05-298322	21708	20	1506426
Fagron	Levothyroxin sod...	14E28-B05-306102	21820	40	20140915
Fagron	Levothyroxin sod...	18G27-B02-352032	24286	40	20180822
Fagron	Levothyroxin sod...	14E28-B05-298322	21708SI	32	1506426
Fagron	Levothyroxin sod...	14E28-B05-306102	21820SI	38	20140915

Validation samples

A total of 280 317 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 *Levothyroxin sodium*. These samples are listed above in the [calibration samples](#) section.
- 74 326 spectra from a total of 1620 batches from further 372 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 [†].

- 226 spectra of 9 reference samples from the substance/substance group *Levothyroxin sodium*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Levothyroxin sodium	14E28-B05-298322	21708 [†]	10
Fagron	Levothyroxin sodium	14E28-B05-306102	21820 [†]	20
Fagron	Levothyroxin sodium	16G25-B99-329080	23191	40
Fagron	Levothyroxin sodium	17J10-B05-348764	24176	40
Fagron	Levothyroxin sodium	14E28-B05-298322	21708SI [†]	15
Fagron	Levothyroxin sodium	14E28-B05-306102	21820SI [†]	15
Fagron	Levothyroxin sodium	16G25-B99-329080	23191SI	24
Fagron	Levothyroxin sodium	17J10-B05-348764	24176SI	30
Fagron	Levothyroxin sodium	18G27-B02-352032	24286SI	32

- 126 666 spectra from a total of 2784 batches from further 781 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*.

- 18 spectra from 5 *Apo-Ident* customers from 2 batches from the substance/substance group *Levothyroxin sodium*.

Supplier	Substance	Batch	Spectra
Fagron	Levothyroxin sodium	16G25-B99-324827	17
Euro OTC	Levothyroxin sodium	17J10-B05-345570	1

- 78 911 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	161	9	74 326
Type B	0	211	15	126 666
Type C	0	16	2	78 911

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	94.7059 % (> 92.9412 %)
Type B	100.0000 % (> 99.9901 %)	93.3628 % (> 92.0354 %)
Type C	100.0000 % (> 99.8817 %)	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
21708	21708	0.00	75.12
21820	21708	17.26	83.78
24286	21708	22.45	87.25

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **L-glutathione**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20366-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

L-glutathione; L-Glutathionum

Special notes

When selecting the *L-glutathione* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *L-glutathione*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	L-glutathione	1102019-02	21788	40	AR-15-FG-008218-01
Euro OTC	L-glutathione	1703008	23143	40	20170327*
Euro OTC	L-glutathione	1808036	24314	40	20180919*

Validation samples

A total of 280 317 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 L-glutathione. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 L-glutathione.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-glutathione	1102019-02	21788 [†]	20
Euro OTC	L-glutathione	1711009	23729	40
Fagron	L-glutathione	18C01-B08-347604	24059	40

- 126 792 spectra from a total of 2786 batches from further 781 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 L-glutathione.

*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
Fagron	L-glutathione	14H21-B02	1
Farmalabor	L-glutathione	P1700811	1

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *L-glutathione* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-glutathione* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	2	0	78 927

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8823 %)	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
21788	21788	0.00	46.73
23143	23143	0.00	47.50
24314	24314	0.00	43.57

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Lidocaine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20942-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lidocaine; Lidocainum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Lidocaine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Lidocaine	13H05-N05	20942	40	1401378
Euro OTC	Lidocaine	1310023-01	21640	40	20131118
Caelo	Lidocaine	13352411	21673	40	20131115
Euro OTC	Lidocaine	1612021	22984	40	20170206*
Fagron	Lidocaine	16F21-B06-327232	23019	40	20160728

Validation samples

A total of 280317 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 *Lidocaine*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 7 reference samples from the substance/substance group *Lidocaine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Lidocaine	1310023-01	21640 [†]	20
Caelo	Lidocaine	13352411	21673 [†]	20
Euro OTC	Lidocaine	1603027	22526	40
Caelo	Lidocaine	162895	22768	40
Caelo	Lidocaine	171831	23632	40
Euro OTC	Lidocaine	1801032	23960	40
Caelo	Lidocaine	180444	24031	40

- 126652 spectra from a total of 2782 batches from further 781 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*.

- 416 spectra from 198 *Apo-Ident* customers from 161 batches from the substance/substance group *Lidocaine*.

Supplier	Substance	Batch	Spectra
Fagron	Lidocaine	12E30-N10	8
Fagron	Lidocaine	11D28-N12	1
Fagron	Lidocaine	12C08-N11	1
Fagron	Lidocaine	11K17-N03	1
Fargon	Lidocaine	12E30-N10	1
Caelo	Lidocaine	5111201	1
Caelo	Lidocaine	12163803	3
Caelo	Lidocaine	12163804	2
Caelo	Lidocaine	11K17-N03	1
Fagron	Lidocaine	6J23-No2	1
Caelo	Lidocaine	12163802	2
Fagron	Lidocaine	12H16-N05	5
Anzag	Lidocaine	12E30-N10	1
Fagron	Lidocaine	12I21-N06	3
Caelo	Lidocaine	9205919	1
Fagron	Lidocaine	12h16-N05	1
Fagron	Lidocaine	12H16-n05	1
Caelo	Lidocaine	12163811	3
Fagron	Lidocaine	12K13-N01	1
Fagron	Lidocaine	12I21N06	1
Caelo	Lidocaine	12163810	1
Fagron	Lidocaine	12/21-N06	2
Sanacorp	Lidocaine	12H16-N05	1
Caelo	Lidocaine	12163813	4
Fagron	Lidocaine	13B27-N04	8
Fagron	Lidocaine	11C09-N07	2
Phönix	Lidocaine	13B27-N04	1
Fagron	Lidocaine	13H05-N05	8
Sanacorp	Lidocaine	12I21-N06	1
Gehe	Lidocaine	13B27-N04	1
Fagron	Lidocaine	12h16n05	1
Caelo	Lidocaine	12294412	9
Caelo	Lidocaine	12294408	2
Noweda	Lidocaine	12H16-N05	1
Fagron	Lidocaine	214U-03584	1
Gehe am 22.01.2014	Lidocaine	13H05-N05	2
Fagron	Lidocaine	13H05-N050171/245	1
Fagron	Lidocaine	1113M-03584	1
Caelo	Lidocaine	12294405	2
Fargon/Phoenix	Lidocaine	13H05-N05	3
Gutenberg-Apotheke	Lidocaine	13J30-B02	1
Fagron	Lidocaine		1
Caesar & Loretz GmbH	Lidocaine	12294412	1
Caelo	Lidocaine	12294405	1
Caelo	Lidocaine	13352403	1
Gehe	Lidocaine	12H16-N05	1
Caelo	Lidocaine	13352406	1
Caelo	Lidocaine	13352408	8
Fagron	Lidocaine	13J30-b02-287639	1
Caelo	Lidocaine	13J30-B02-292221	1
Fagron	Lidocaine	13J30-B02-292221	5
Fagron	Lidocaine	13J30-B02-287640	1
Henry Lamotte Oils GmbH	Lidocaine		1
Fagron	Lidocaine	13J30-B02	6
PHOENIX 22.08.2014	Lidocaine		2

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Supplier	Substance	Batch	Spectra
Fagron	Lidocaine	13J30-B02-287641	6
Fagron	Lidocaine	13J30-B02-292219	2
Caelo	Lidocaine	13352405	1
PHOENIX 22.08.2014	Lidocaine	13J30-B02-287640	1
Caelo	Lidocaine	13352411	6
GEHE 02.12.2014	Lidocaine	13J30-B02-292220	1
Fagron	Lidocaine	5122014A	1
Fagron	Lidocaine	13J30-B02-292220	2
Fagron	Lidocaine	1014I-07006	1
Fagron	Lidocaine	13j30B02292219	1
Fagron	Lidocaine	14E13-B05-295549	3
Caelo	Lidocaine	133524	1
Caelo	Lidocaine	13352413	3
Fagron	Lidocaine	14E13-B05	2
Fagron	Lidocaine	13E28-B40-289433	1
Fagron	Lidocaine	14E13-B05-295550	2
Gehe Kassel	Lidocaine	14E13-B05-295550	1
Caelo	Lidocaine	14299301	2
Caelo	Lidocaine	13352414	2
Gehe	Lidocaine	14E13-B05-295552	1
Caelo	Lidocaine	14299303	2
Caelo	Lidocaine	14299305	2
Fagron	Lidocaine	15A15-B01-304282	4
Caelo	Lidocaine	13352415	3
Fagron	Lidocaine	15A15-B01-304283	2
Fagron	Lidocaine	14E13-B05-295552	3
Caelo	Lidocaine	15212001	2
Caelo	Lidocaine	15212003	3
Phönix Gotha	Lidocaine	15A15-B01-304284	1
Fagron	Lidocaine	15A15B01304284	1
Caelo	Lidocaine	15212002	3
Caelo	Lidocaine	15A15-B01-304284	2
Fagron	Lidocaine	15d23-b08-309882	1
Fargron	Lidocaine	14E13-B05-295552	1
Fagron	Lidocaine	15A15-B01-304284	6
Fagron	Lidocaine	15D23-B08-312058	10
Fagron	Lidocaine	15D23-B08-309882	1
Caelo	Lidocaine	15332302	3
Euro OTC	Lidocaine	1310023-02	3
Caelo	Lidocaine	1512003	1
Fagron	Lidocaine	515M-07006	1
Fagron	Lidocaine	15A15-B01	1
Moehs BCN S.L. / Noweda	Lidocaine	15332305	1
Fagron	Lidocaine	15H27-B07	1
Rondell Apotheke	Lidocaine	15332304	1
Fagron	Lidocaine	15D23-B08	1
Caelo	Lidocaine	15332306	3
Fagron	Lidocaine	15D23-B08312058	1
Fagron	Lidocaine	15D23B08311708	1
Caelo	Lidocaine	8629595	1
Phoenix	Lidocaine	15332305	1
Fagron	Lidocaine	15H27-B07-316784	1
Fagron	Lidocaine	15d23-b08-312058	2
Caelo	Lidocaine	15332305	2
Fagro/Gehe	Lidocaine	15a15b01304284	1
Fagron	Lidocaine	15H27-B07-315483	2
Caelo	Lidocaine	15332309	2
Caelo	Lidocaine	16087703	1
Caelo	Lidocaine	15332310	3
Fagron	Lidocaine	16A28-B06-320059	2

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Supplier	Substance	Batch	Spectra
Fagron	Lidocaine	15h27-b05-318310	1
Caelo	Lidocaine	16A28-B06-320059	1
Caelo	Lidocaine	15D23-B08	1
Caelo	Lidocaine	16087702	1
Caelo	Lidocaine	15332314	2
Alliance	Lidocaine	15H27-B07-318310	1
Caelo	Lidocaine	16087707	7
Caelo	Lidocaine	16087704	7
AHD	Lidocaine	15332314	1
Fagron	Lidocaine	15H27-B07-318310	2
Fagron	Lidocaine	15D23-B08309882	1
Caelo	Lidocaine	15332303	1
Alte Apotheke	Lidocaine	16A28B06-321297	1
Fagron	Lidocaine	LDB/116049	1
Caesar&Loretz,Phönix,06...	Lidocaine	15332314	1
Caelo	Lidocaine	16087710	2
Caelo	Lidocaine	16087709	1
Caelo	Lidocaine	16087711	8
Fagron	Lidocaine	16F21-B06-323670	10
Caelo	Lidocaine	16087712	4
Fagron	Lidocaine	16F21-B06-323669	5
Fagron	Lidocaine	1116E-07006	1
Caelo	Lidocaine	160877708	1
Caelo	Lidocaine	16289502	6
Fagron	Lidocaine	16F21-B06-325934	1
Caelo	Lidocaine	16289503	4
Caelo	Lidocaine	16087708	1
Faron/Alliance	Lidocaine	16F21-B06-323670	2
Euro OTC	Lidocaine	1603027-01	2
Fagron	Lidocaine	16F21B06325934	1
Caelo	Lidocaine	16289504	2
Caelo	Lidocaine	16289507	2
Allianz Healthcare	Lidocaine	8565960	1
GEHE	Lidocaine	16289503	1
Fagron	Lidocaine	16F21-B06	2
Fagron	Lidocaine	16F21-B06-327232	2
Caelo	Lidocaine	15H27-B07-318310	1
Caelo	Lidocaine	16F21-B06-323670	1
Caelo	Lidocaine	15H-B07-318310	1
Fagron	Lidocaine	5742	1
Sanacorp	Lidocaine	1603027-02	1
Ebert-Jacobi	Lidocaine	16289504	1
Kehr	Lidocaine	16F21-B06-328421	1
Caelo	Lidocaine	16F21-B06-328421	2
Fagron	Lidocaine	16F21-B06-328421	5
Fagron	Lidocaine	16F21-B06-328421	1
Caelo	Lidocaine	16289508	10
GEHE	Lidocaine	16F21-B06-328421	1
Fagron	Lidocaine	16F21B06332251	1
Caelo	Lidocaine	16F21-806-333787	1
Fagron	Lidocaine	16F21-B06-332253	1
Fagron	Lidocaine	16F21	2
Kehr	Lidocaine	16F21-B06-332251	1
Caelo	Lidocaine	1629508	1
Caelo	Lidocaine	17183102	2
Caelo	Lidocaine	17183108	5
Caesar&Loretz GmbH	Lidocaine	16289502	1
Fagron	Lidocaine	16F21-B06-333788	1
Fagron	Lidocaine	16F21-B06-332253	3
Caelo	Lidocaine	17183105	1

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Supplier	Substance	Batch	Spectra
Kehr	Lidocaine	17G03-B08-338284	1
Caelo	Lidocaine	17183109	1
Caelo	Lidocaine	17183103	2
Fagron	Lidocaine	17G03-B08	2
Caelo	Lidocaine	17348502	1
Fagron	Lidocaine	17G03-B08-338286	1
Fagron	Lidocaine	71-18	1
Caelo	Lidocaine	17G03-B08	1
Caelo	Lidocaine	18041812	1
Fagron	Lidocaine	17G03-B08-341308	2
Caelo	Lidocaine	17348503	3
Fagron	Lidocaine	17G03-B08-343251	1
Euro OTC	Lidocaine	161202102	1
Fagron	Lidocaine	17K23-B04-343250	1
Caelo	Lidocaine	17G03B08341308	1
Caelo	Lidocaine	1783109	1
Euro OTC	Lidocaine	1612021-01	1
Fagron	Lidocaine	17K23-B04-345215	1
Caelo	Lidocaine	17348503	1
Fagron	Lidocaine	17K23-B04-347475	3
Fagron	Lidocaine	17K23B04347473	1
Fagron	Lidocaine	17G03-B08-341306	1
Sanacorp	Lidocaine	17183109	1
Fagron	Lidocaine	17K23-B04-350189	3
Fagron	Lidocaine	17K23-B04-350541	1
Fagron	Lidocaine	17G23-B04-350541	1
Caelo	Lidocaine	17K23-B04-350543	1

- 78 513 spectra from 565 *Apo-Ident* customers from a total of 25 978 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Lidocaine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lidocaine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	240	0	126 652
Type C	0	415	1	78 513

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.8817 %)	99.7596 % (> 99.0385 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20942	20942	0.00	45.65
21640	22984	6.64	45.21
21673	22984	18.68	45.97
22984	22984	0.00	42.26
23019	22984	3.03	39.85

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Lidocaine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20093-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lidocaine hydrochloride; Lidocaini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Lidocaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lidocaine hydroc...	12135511	20882	40	AR-15-FG-008867-01
Euro OTC	Lidocaine hydroc...	1403025-02	21613	40	20140516
Euro OTC	Lidocaine hydroc...	1411010	21770	40	0000009260

Validation samples

A total of 280 317 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 *Lidocaine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Lidocaine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Lidocaine hydrochloride	1403025-02	21613 [†]	20
Euro OTC	Lidocaine hydrochloride	1411010	21770 [†]	20
Euro OTC	Lidocaine hydrochloride	1606024	22702	40
Caelo	Lidocaine hydrochloride	162222	22771	40
Caelo	Lidocaine hydrochloride	152995	22772	40
Euro OTC	Lidocaine hydrochloride	1612015	22980	40
Caelo	Lidocaine hydrochloride	172048	23687	40
Caelo	Lidocaine hydrochloride	172923	23807	40
Euro OTC	Lidocaine hydrochloride	1808031	24326	40

- 126 572 spectra from a total of 2780 batches from further 781 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.

- 1000 spectra from 352 *Apo-Ident* customers from 221 batches from the substance/substance group *Lidocaine hydrochloride*.

[†]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	Lidocaine hydrochloride	1103034-01	2
Caelo	Lidocaine hydrochloride	11302906	3
Caelo	Lidocaine hydrochloride	10320707	2
Caelo	Lidocaine hydrochloride	10320703	1
Fagron	Lidocaine hydrochloride	11L09-N09	2
Euro OTC	Lidocaine hydrochloride	1108017-02	7
Gehe	Lidocaine hydrochloride	12C05-N02	2
Fagron	Lidocaine hydrochloride	8F26-N07	1
Caelo	Lidocaine hydrochloride	10320704	1
Caelo	Lidocaine hydrochloride	25091202	1
Caelo	Lidocaine hydrochloride	11091203	1
Euro OTC	Lidocaine hydrochloride	LID-20-11-001	2
Euro OTC	Lidocaine hydrochloride	1202035-01	24
Noweda	Lidocaine hydrochloride	1108017-02	1
Caelo	Lidocaine hydrochloride	12176101	8
Caelo	Lidocaine hydrochloride	120203501	1
Caelo	Lidocaine hydrochloride	12135503	2
Euro OTC	Lidocaine hydrochloride	1202034-01	2
Fagron	Lidocaine hydrochloride	12c05-N02	1
Caelo	Lidocaine hydrochloride	11302904	1
Caelo	Lidocaine hydrochloride	5211E-01775	1
Caelo	Lidocaine hydrochloride	12135504	3
Caelo	Lidocaine hydrochloride	12176102	8
Finze	Lidocaine hydrochloride	1202035-01	1
Sanacorp	Lidocaine hydrochloride	1202035-01	3
Euro OTC	Lidocaine hydrochloride	20131010-4	1
EuRho	Lidocaine hydrochloride	1108017-01	3
Caelo	Lidocaine hydrochloride	10320717	1
Caelo	Lidocaine hydrochloride	12176103	8
Fagron	Lidocaine hydrochloride	12H09-N08	2
Gehe	Lidocaine hydrochloride	1190313	1
Fagron	Lidocaine hydrochloride	12E14-N04	2
Caelo	Lidocaine hydrochloride	11302902	2
Caelo	Lidocaine hydrochloride	11302905	1
Caelo	Lidocaine hydrochloride	2051301	1
Caelo	Lidocaine hydrochloride	12135509	4
A.H.D.	Lidocaine hydrochloride	1202035-02	1
Caelo	Lidocaine hydrochloride	12176109	2
Caelo	Lidocaine hydrochloride	10320719	1
Phönix	Lidocaine hydrochloride	12176103	1
Euro OTC	Lidocaine hydrochloride	2213U01775	1
Euro OTC	Lidocaine hydrochloride	1202035-02	35
Caelo	Lidocaine hydrochloride	12135508	5
Caelo	Lidocaine hydrochloride	1202035-02	5
Euro OTC	Lidocaine hydrochloride	1202035-1	1
Fiebig 04.7.13 EK 4,54	Lidocaine hydrochloride	12135511	1
Caelo	Lidocaine hydrochloride	12135511	2
Caelo	Lidocaine hydrochloride	26071303	1
Fagron	Lidocaine hydrochloride	13F07-N06	7
Euro OTC	Lidocaine hydrochloride	2810029-01	1
Euro OTC	Lidocaine hydrochloride	1202035/02	1
Fagron	Lidocaine hydrochloride	12C05-N02	1
Gehe	Lidocaine hydrochloride	1202035-02	1
Caesar&Loretz GmbH/Anzag	Lidocaine hydrochloride	13118803	2
Caelo	Lidocaine hydrochloride	13118802	2
Caelo	Lidocaine hydrochloride	13118807	6
Caelo	Lidocaine hydrochloride	13118803	5
Caelo	Lidocaine hydrochloride	AKD14	1
Euro OTC	Lidocaine hydrochloride	1202035-03	11
Euro OTC	Lidocaine hydrochloride	120203502	3

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Supplier	Substance	Batch	Spectra
Caelo	Lidocaine hydrochloride	4111302	1
Euro OTC	Lidocaine hydrochloride	1010024-01	2
Euro OTC	Lidocaine hydrochloride	2805016-01	1
Phönix	Lidocaine hydrochloride	1202035-03	1
Caelo	Lidocaine hydrochloride	13118808	4
Caerlo	Lidocaine hydrochloride	13118807	1
Fagron	Lidocaine hydrochloride	9B3M1L2Fo118	1
Euro OTC	Lidocaine hydrochloride	1108017-01	4
Euro OTC	Lidocaine hydrochloride	1202035	1
Caelo	Lidocaine hydrochloride	1202035-03	1
Euro OTC	Lidocaine hydrochloride	1004040-01	1
Caelo	Lidocaine hydrochloride	23011403	1
Caelo	Lidocaine hydrochloride	1202035	1
Fagron	Lidocaine hydrochloride	13F07N06	1
PHOENIX am 12.02.2014	Lidocaine hydrochloride	1202035-02	1
Caelo	Lidocaine hydrochloride	13118812	3
Sanacorp	Lidocaine hydrochloride	13118807	1
Hedinger/Ebert	Lidocaine hydrochloride	13118807	1
Noweda	Lidocaine hydrochloride	1202035-03	1
Anzag	Lidocaine hydrochloride	1202035-03	1
Konduskar/Phönix	Lidocaine hydrochloride	1202035-03	1
Caelo	Lidocaine hydrochloride	13118811	2
Caelo	Lidocaine hydrochloride	26041401	1
Caelo	Lidocaine hydrochloride	1912M-01775	1
Caelo	Lidocaine hydrochloride	13343001	2
Caesar & Loretz GmbH	Lidocaine hydrochloride	13343002	1
Fagron	Lidocaine hydrochloride	13L18-B11-286901	1
Moehs Catalana, S.L./Ph...	Lidocaine hydrochloride		1
Caelo	Lidocaine hydrochloride	13343002	3
Caelo	Lidocaine hydrochloride		1
Europ Ots Pharma	Lidocaine hydrochloride	1403025-01	1
Euro OTC	Lidocaine hydrochloride	1403025-01	17
EuRho	Lidocaine hydrochloride	140302501	1
Caelo	Lidocaine hydrochloride	13343004	7
Caelo	Lidocaine hydrochloride	13343003	5
01.07.14	Lidocaine hydrochloride	13343004	1
Fagron	Lidocaine hydrochloride	9E08-N03	1
Euro OTC	Lidocaine hydrochloride	140302501	2
Anzag	Lidocaine hydrochloride	1403025-01	1
Fagron	Lidocaine hydrochloride	14B12-B03-292214	9
Caelo	Lidocaine hydrochloride	13343008	4
PHOENIX 17.06.2014	Lidocaine hydrochloride	1403025-01	1
Caelo	Lidocaine hydrochloride	13343007	12
Caelo	Lidocaine hydrochloride	24071401	1
Caolo	Lidocaine hydrochloride	13343008	1
Caelo	Lidocaine hydrochloride	1403025-02	2
sana	Lidocaine hydrochloride	1403025-02	1
Caelo	Lidocaine hydrochloride	5113E-01775	1
Fagron	Lidocaine hydrochloride	14E13-B06-294975	5
Euro OTC	Lidocaine hydrochloride	1403025-02	12
Caelo	Lidocaine hydrochloride	16101407	1
Caelo	Lidocaine hydrochloride	13343012	16
Caelo	Lidocaine hydrochloride	13343011	3
Euro OTC	Lidocaine hydrochloride		3
Fagron	Lidocaine hydrochloride	1202035-02	1
Fagron	Lidocaine hydrochloride	14e13-b06-294975	1
Anzag	Lidocaine hydrochloride	14B12-B03-292214	1
Caelo	Lidocaine hydrochloride	13343014	5
Caelo	Lidocaine hydrochloride	12021503	1
Euro OTC	Lidocaine hydrochloride	1411010-01	31

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Supplier	Substance	Batch	Spectra
Caelo	Lidocaine hydrochloride	13343017	5
Euro OTC	Lidocaine hydrochloride	1403025-03	1
Fagron	Lidocaine hydrochloride	14J07-B04-299433	3
Euro OTC	Lidocaine hydrochloride	140302502	2
Caelo	Lidocaine hydrochloride	13343015	2
Mahendra Chem./ Phönix ...	Lidocaine hydrochloride	1411010-01	1
Caelo	Lidocaine hydrochloride	1814U-01775	1
Euro OTC	Lidocaine hydrochloride	140415A	1
Alliance health	Lidocaine hydrochloride	14B12-B03-292214	1
Caelo	Lidocaine hydrochloride	18041501	1
Fagron	Lidocaine hydrochloride	4612Q-01775	1
Sanacorp	Lidocaine hydrochloride	14J07-B04-299434	2
Euro OTC	Lidocaine hydrochloride	141101-01	1
Anzag	Lidocaine hydrochloride	1411010-01	1
Euro OTC	Lidocaine hydrochloride	1401010-01	1
Euro OTC	Lidocaine hydrochloride	141101001	4
Caelo	Lidocaine hydrochloride	1411010-01	2
Caelo	Lidocaine hydrochloride	280501	1
Euro OTC	Lidocaine hydrochloride	14110101-01	1
Fagron	Lidocaine hydrochloride	14e13-b06-294973	1
Gehe	Lidocaine hydrochloride	1411010-01	1
Caelo	Lidocaine hydrochloride	14254001	3
Euro OTC	Lidocaine hydrochloride	1411010-01Mg25g	1
Mahendra Chem.	Lidocaine hydrochloride	1411010-01	1
Euro/Phönix	Lidocaine hydrochloride	141101010-01	1
Euro OTC	Lidocaine hydrochloride	1411010-02	22
Caelo	Lidocaine hydrochloride	13343019	4
Phönix Gotha	Lidocaine hydrochloride	1411010-02	1
Fagron	Lidocaine hydrochloride	14J07-B04-299434	2
Euro OTC	Lidocaine hydrochloride	141101002	3
Caelo	Lidocaine hydrochloride	14110101	1
Caesar u Loretz	Lidocaine hydrochloride	13343017	1
Caelo	Lidocaine hydrochloride	13343016	1
Caelo	Lidocaine hydrochloride	15215302	2
Caelo	Lidocaine hydrochloride	29081503	1
Caelo	Lidocaine hydrochloride	15215301	6
Caelo	Lidocaine hydrochloride	14J20-B05-303133	1
Fagron	Lidocaine hydrochloride	13218-B11	1
Euro OTC	Lidocaine hydrochloride	1411010-2	1
Caelo	Lidocaine hydrochloride	14J20-B05-303131	1
Caelo	Lidocaine hydrochloride	15215304	3
Caelo	Lidocaine hydrochloride	1521304	1
Euro OTC	Lidocaine hydrochloride	1505023-01	53
Fagron	Lidocaine hydrochloride	14J20-B05-303133	2
Noweda	Lidocaine hydrochloride	141101002	1
Euro OTC	Lidocaine hydrochloride	1411010-02Mg50g	1
Euro OTC	Lidocaine hydrochloride	150502301	2
ACM	Lidocaine hydrochloride	KNC1247J15	1
EuRho	Lidocaine hydrochloride	1505023-01	3
Caesar & Loretz GmbH	Lidocaine hydrochloride	15215201	1
Caelo	Lidocaine hydrochloride	15215308	2
Bombastus	Lidocaine hydrochloride	15215301	1
Euro	Lidocaine hydrochloride	1505023-01	2
Caelo	Lidocaine hydrochloride	15215201	3
Caesar&Loretz GmbH /Anzag	Lidocaine hydrochloride	15215303	1
Fagron	Lidocaine hydrochloride	14J20-B05-303131	1
Euro OTC	Lidocaine hydrochloride	141101	1
Caelo	Lidocaine hydrochloride	15215310	9
Caelo	Lidocaine hydrochloride	1505023-01	6
Fagron	Lidocaine hydrochloride	14j20-b05-303133	1

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Supplier	Substance	Batch	Spectra
Rondell Apotheke	Lidocaine hydrochloride	15215308	1
Fagron	Lidocaine hydrochloride	1505023-01	2
Caelo	Lidocaine hydrochloride	15215311	3
Caelo	Lidocaine hydrochloride	15215303	2
Caelo	Lidocaine hydrochloride	15215309	2
Fagron	Lidocaine hydrochloride	15215311	2
Sanacorp	Lidocaine hydrochloride	15215309	1
Caelo	Lidocaine hydrochloride	15299503	9
Caelo	Lidocaine hydrochloride	1515I-01775	1
Caelo	Lidocaine hydrochloride	168020-0003	1
Fagron	Lidocaine hydrochloride	15/17-B01-316805	3
Caelo	Lidocaine hydrochloride	1517-B01-315828	1
Euro OTC	Lidocaine hydrochloride	1505023-02	16
Gehe	Lidocaine hydrochloride	15215304	1
EuRho	Lidocaine hydrochloride	1505023-02	1
Euro OTC	Lidocaine hydrochloride	1505023-03	12
Caelo	Lidocaine hydrochloride	15299506	3
Caelo	Lidocaine hydrochloride	1505023-03	2
Euro OTC	Lidocaine hydrochloride	23081601	1
Euro/Alliance Healthcare	Lidocaine hydrochloride	150523-01	1
Fagron	Lidocaine hydrochloride	15/17-B01316805	1
Fagron	Lidocaine hydrochloride	15117-B01-315828	2
Euro OTC	Lidocaine hydrochloride	1606024-01	42
Euro OTC	Lidocaine hydrochloride	160602401	2
Sanacorp	Lidocaine hydrochloride	150502302	1
Phönix	Lidocaine hydrochloride	1606024-01	1
Caelo	Lidocaine hydrochloride	160719LC	1
Mahendra Chem./Noweda	Lidocaine hydrochloride	1505023	1
Ensbona/ Sanacorp	Lidocaine hydrochloride	1606024-01	1
Bombastus	Lidocaine hydrochloride	1606024-01	6
phönix	Lidocaine hydrochloride	1505023-03	1
Caelo	Lidocaine hydrochloride	15215312	6
Swati / Noweda	Lidocaine hydrochloride	1606024-01	1
Swati/Noweda	Lidocaine hydrochloride	LDH/116007	1
ALH	Lidocaine hydrochloride	1606024-01	1
Fagron	Lidocaine hydrochloride	15I17-B01-316805	2
Caelo	Lidocaine hydrochloride	15299509	2
Caelo	Lidocaine hydrochloride	1606024-01	15
Alte Apotheke	Lidocaine hydrochloride	1606024-01	2
Fargon GmbH & Co.KG	Lidocaine hydrochloride	15/17-B01-316805	1
Euro OTC	Lidocaine hydrochloride	1606021-01	1
Caelo	Lidocaine hydrochloride	15299514	6
Caelo	Lidocaine hydrochloride	15299513	7
Fagron	Lidocaine hydrochloride	15299513	1
Fargon GmbH & Co.KG	Lidocaine hydrochloride	16C09-B03-322144	2
Caelo	Lidocaine hydrochloride	15299516	4
Caelo	Lidocaine hydrochloride	16222202	2
siehe Protokoll	Lidocaine hydrochloride	1606024-01	1
Fagron	Lidocaine hydrochloride	16C09-B03	1
Caelo	Lidocaine hydrochloride	1606024-02	4
Caelo	Lidocaine hydrochloride	152951602714117	1
Caelo	Lidocaine hydrochloride	1505023-02	1
Fagron	Lidocaine hydrochloride	16C09-B03-322144	4
Caelo	Lidocaine hydrochloride	16222203	7
Euro OTC	Lidocaine hydrochloride	1066024-01	1
Euro OTC	Lidocaine hydrochloride	1606024-02	31
Symbiotica	Lidocaine hydrochloride	1606024-02	1
Gehe	Lidocaine hydrochloride	15299516	1
Gehe	Lidocaine hydrochloride	1606024-02	1
Fagron	Lidocaine hydrochloride	16C09-B03-319230	1

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Supplier	Substance	Batch	Spectra
Phoenix	Lidocaine hydrochloride	16C09-B03-322144	1
Fagron	Lidocaine hydrochloride	16J24-B15-329421	1
Caelo	Lidocaine hydrochloride	4051703	1
Caelo	Lidocaine hydrochloride	1606024	1
Frago/Noweda	Lidocaine hydrochloride	6108-05-0	1
Sanacorp	Lidocaine hydrochloride	15215312	1
Noweda	Lidocaine hydrochloride	16222207	2
Caelo	Lidocaine hydrochloride	3071711	1
Euro OTC	Lidocaine hydrochloride	1600024-02	1
Kehr	Lidocaine hydrochloride	1606024-02	1
Caelo	Lidocaine hydrochloride	16222207	2
Euro OTC	Lidocaine hydrochloride	1612015-01	13
phönix	Lidocaine hydrochloride	16222207	2
Caelo	Lidocaine hydrochloride	16222208	3
Caelo	Lidocaine hydrochloride	1230817/160602402	1
Euro OTC	Lidocaine hydrochloride	1606024-03	8
Fagron	Lidocaine hydrochloride	17A16-B07-333010	4
GEHE	Lidocaine hydrochloride	1612015-01	1
GEHE	Lidocaine hydrochloride	1606024-02	1
Euro OTC	Lidocaine hydrochloride	1140917/160602403	1
Caelo	Lidocaine hydrochloride	812-16001	1
Caelo	Lidocaine hydrochloride	16222214	4
ACM	Lidocaine hydrochloride	KNC0625J17	1
Klenk	Lidocaine hydrochloride	1612015-01	2
GEHE	Lidocaine hydrochloride	16222214	1
Caelo	Lidocaine hydrochloride	1606024-03	1
EuRho	Lidocaine hydrochloride	1612015-01	1
Noweda	Lidocaine hydrochloride	1606024-02	1
Caesar & Loretz	Lidocaine hydrochloride	1612015-01	2
Noweda	Lidocaine hydrochloride	16222214	1
Euro OTC	Lidocaine hydrochloride	16112015-01	2
Caelo	Lidocaine hydrochloride	1612015-01	3
Euro OTC	Lidocaine hydrochloride	171106LHC/1606024-03	1
Caelo	Lidocaine hydrochloride	4111703	1
Apo-Ident, Phönix, 7.11...	Lidocaine hydrochloride	1612015-01	1
Caelo	Lidocaine hydrochloride	17204803	4
Euro OTC	Lidocaine hydrochloride	12020351612015-01	1
Caelo	Lidocaine hydrochloride	6121706	1
Fagron	Lidocaine hydrochloride	LDH/116037	2
Euro OTC	Lidocaine hydrochloride	1612015-02	25
Caelo	Lidocaine hydrochloride	17204804	11
ALH/EuRho	Lidocaine hydrochloride	1612015-01	1
Fagron	Lidocaine hydrochloride	218I-01775	1
Euro/ Anzag	Lidocaine hydrochloride	1606024-03	1
Anzag	Lidocaine hydrochloride	17204804	2
Euro OTC	Lidocaine hydrochloride	180220L/1612015-01	1
Caelo	Lidocaine hydrochloride	1612015-02	4
Fagron	Lidocaine hydrochloride	1612015-01	1
Fagron	Lidocaine hydrochloride	1612015-02	2
Euro/Phönix	Lidocaine hydrochloride	1612015-01	1
Sanacorp	Lidocaine hydrochloride	17204804	1
Euro OTC	Lidocaine hydrochloride	ldh/116023	1
Kehr	Lidocaine hydrochloride	1612015-01	1
EuRho/Phoenix	Lidocaine hydrochloride	1612015-01	1
Caelo	Lidocaine hydrochloride	17204810	1
Caelo	Lidocaine hydrochloride	17292304	5
Fagron	Lidocaine hydrochloride	17A16-B07-331959	1
Gehe	Lidocaine hydrochloride	1612015-02	1
Caelo	Lidocaine hydrochloride	26051802	1
Fagron	Lidocaine hydrochloride	17G10-B08-342287	1

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Supplier	Substance	Batch	Spectra
Caelo	Lidocaine hydrochloride	17292302	2
Euro OTC	Lidocaine hydrochloride	1612015-03	6
Gehe/Euro	Lidocaine hydrochloride	1612015-02	1
Caesar & Lorenz GmbH	Lidocaine hydrochloride	16222208	1
Kehr	Lidocaine hydrochloride	1612015-02	1
Euro OTC	Lidocaine hydrochloride	1612015-04	7
Fagron	Lidocaine hydrochloride	17G10-B08-346659	1
Caelo	Lidocaine hydrochloride	17292310	1
Noweda/EuRo	Lidocaine hydrochloride	1612015-03	1
Noweda	Lidocaine hydrochloride	1812015-04	1
Caelo	Lidocaine hydrochloride	17292308	2
Allianz	Lidocaine hydrochloride	17292308	1
Gehe	Lidocaine hydrochloride	LDH/116023	1
Caelo	Lidocaine hydrochloride	1612015-03	1
Fagron	Lidocaine hydrochloride	18B23-B03-348590	2
Euro OTC	Lidocaine hydrochloride	1612015	1
Caelo	Lidocaine hydrochloride	17292307	1
Caelo	Lidocaine hydrochloride	1792313	1
Euro OTC	Lidocaine hydrochloride	16112015-04	1
Euro OTC	Lidocaine hydrochloride	1808031-01	6
Caelo	Lidocaine hydrochloride	17292311	1
Caelo	Lidocaine hydrochloride	28111812	1
Fagron	Lidocaine hydrochloride	18B23-B03-352117	2
Caelo	Lidocaine hydrochloride	17292313	1
Kehr	Lidocaine hydrochloride	1612015-03	1
Caelo	Lidocaine hydrochloride	1729313	1
Caelo	Lidocaine hydrochloride	2021903	1

- 77 929 spectra from 565 *Apo-Ident* customers from a total of 25 921 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Lidocaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lidocaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	320	0	126 572
Type C	0	935	65	77 929

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.8817 %)	93.5000 % (> 93.2000 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20882	20882	0.00	42.71
21613	20882	7.79	41.43
21770	21770	0.00	42.48

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **L-isoleucine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21045-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

L-isoleucine; L-Isoleucinum

Special notes

When selecting the *L-isoleucine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *L-isoleucine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	L-isoleucine	13E02-B01-286930	21045	40	1403154
Fagron	L-isoleucine	13E02-B01	21332	40	20130621
Euro OTC	L-isoleucine	1604057	22566	40	20160601*
Euro OTC	L-isoleucine	1704022	23386	40	20170612*

Validation samples

A total of 280317 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 *L-isoleucine*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 7 reference samples from the substance/substance group *L-isoleucine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-isoleucine	L1211010-02	21535	60
Euro OTC	L-isoleucine	L1211010-02	21581	60
Euro OTC	L-isoleucine	1611007	22869	40
Euro OTC	L-isoleucine	1708027	23702	40
Euro OTC	L-isoleucine	1711034	23869	40
Euro OTC	L-isoleucine	1803019	24080	40
Euro OTC	L-isoleucine	1805013	24115	40

- 126572 spectra from a total of 2783 batches from further 781 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.

- 11 spectra from 6 *Apo-Ident* customers from 9 batches from the substance/substance group *L-isoleucine*.

Supplier	Substance	Batch	Spectra
Fagron	L-isoleucine	12080167	1
Fagron	L-isoleucine	13A22-N03	1
Fagron	L-isoleucine	13E02-B01-286930	1
Fagron	L-isoleucine	14D08-B02-296089	2
Fagron	L-isoleucine	16H24-B03-331739	1
Fagro WE:19.05.16 EK:64...	L-isoleucine	15A14-B09-314881	1
Fagron	L-isoleucine	17H14-B04-339008	2
Synop WE:18.12.17 E.K:...	L-isoleucine	17H14-B04-339009	1
Euro OTC	L-isoleucine	1708027-01	1

- 78 918 spectra from 565 *Apo-Ident* customers from a total of 26 128 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *L-isoleucine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-isoleucine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	311	9	126 572
Type C	0	10	1	78 918

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	97.1875 % (> 96.2500 %)
Type C	100.0000 % (> 99.8818 %)	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
21045	21045	0.00	37.28
21332	22566	3.56	35.59
22566	22566	0.00	32.42
23386	23386	0.00	32.60

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Lithium orotate monohydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21055-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lithium orotate monohydrate; Lithii orotas monohydricim

Special notes

When selecting the *Lithium orotate monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Lithium orotate monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Lithium orotate ...	13J04-N01	21055	40	1405616
Fagron	Lithium orotate ...	13I09-B04-290311	21688	40	20130927
Fagron	Lithium orotate ...	15F25-B01-315219	22502	40	20150716

Validation samples

A total of 280 317 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 *Lithium orotate monohydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Lithium orotate monohydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Lithium orotate monohydrate	13I09-B04-290311	21688 [†]	20
Fagron	Lithium orotate monohydrate	16D15-B08-321402	23269	40
Fagron	Lithium orotate monohydrate	18A19-B12-347442	24111	40

- 126 792 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Lithium orotate monohydrate*.

Supplier	Substance	Batch	Spectra
Pfannenschmidt	Lithium orotate monohydrate	ORL00212	1
Fagron	Lithium orotate monohydrate	13J04-N01	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*.

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Lithium orotate monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lithium orotate monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	2	0	78 927

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8823 %)	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
22502	21055	4.92	60.07
21055	21055	0.00	59.05
21688	21055	1.48	59.58

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **L-leucine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20970-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

L-leucine; Leucinum

Special notes

When selecting the *L-leucine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *L-leucine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	L-leucine	13J09-N03	20970	40	1402431
Euro OTC	L-leucine	1302013-01	21612	40	20130320
Euro OTC	L-leucine	1601032	22380	40	20160308*
Fagron	L-leucine	15D09-B06-322249	23199	40	20151030

Validation samples

A total of 280 317 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 *L-leucine*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *L-leucine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-leucine	1302013-01	21612 [†]	20
Euro OTC	L-leucine	1708010	23607	40

- 126 832 spectra from a total of 2787 batches from further 781 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 3 batches from the substance/substance group *L-leucine*.

*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
Fargon	L-leucine	8160410903	1
Euro OTC	L-leucine	1312032-01	1
Euro OTC	L-leucine	1708010-01	2

- 78 925 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *L-leucine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-leucine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	60	0	126 832
Type C	0	4	0	78 925

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.8820 %)	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
23199	22380	7.18	73.54
20970	20970	0.00	66.96
21612	20970	7.55	70.95
22380	22380	0.00	71.21

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **L-malic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22357-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

L-malic acid; Acidum-(L)-malicum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *L-malic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	L-malic acid	15J09-B03-313987	22357	40	9346
Fagron	L-malic acid	16J06-B98-327269	23107	40	20161117

Validation samples

A total of 280 317 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 *L-malic acid*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *L-malic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	L-malic acid	15J09-B03-313987	22357 [†]	20
Fagron	L-malic acid	15J09-B03-313987	22612	40
Fagron	L-malic acid	15J09-B03-313987	22730	40
Fagron	L-malic acid	16J06-B98-327269	23222	40
Fagron	L-malic acid	17E23-B03-335458	23762	40

- 126 712 spectra from a total of 2786 batches from further 781 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 *L-malic acid*.

[†]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*.

- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *L-malic 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 *L-malic 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	74 416
Type B	0	180	0	126 712
Type C	0	0	0	78 929

The substance/substance group *L-malic 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 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	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
22357	22357	0.00	102.45
23107	22357	2.30	101.18

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **L-phenylalanine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21661-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

L-phenylalanine; Phenylalaninum

Special notes

When selecting the *L-phenylalanine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *L-phenylalanine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	L-phenylalanine	14088304	21661	40	1501656
Euro OTC	L-phenylalanine	1212014-03	21681	40	20130111
Euro OTC	L-phenylalanine	1704003	23173	40	20170425*

Validation samples

A total of 280 317 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 *L-phenylalanine*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *L-phenylalanine*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	L-phenylalanine	14088304	21661 [†]	20
Euro OTC	L-phenylalanine	1212014-03	21681 [†]	20
Euro OTC	L-phenylalanine	1409013-02	23024	40
Fagron	L-phenylalanine	17B13-B03-343288	23936	40
Euro OTC	L-phenylalanine	1808022	24198	40

- 126 732 spectra from a total of 2784 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 13 spectra from 5 *Apo-Ident* customers from 2 batches from the substance/substance group *L-phenylalanine*.

*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	L-phenylalanine	1409013-02	12
Euro OTC	L-phenylalanine	1704003-02	1

- 78 916 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *L-phenylalanine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-phenylalanine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	156	4	126 732
Type C	0	12	1	78 916

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	97.5000 % (> 95.6250 %)
Type C	100.0000 % (> 99.8818 %)	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
23173	23173	0.00	58.75
21661	21661	0.00	50.29
21681	23173	10.06	58.73

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **L-proline**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21034-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

L-proline; Prolinum

Special notes

When selecting the *L-proline* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *L-proline*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	L-proline	15D13-B02-308152	22270	40	1704059
Euro OTC	L-proline	1606010	22677	40	20160714*
Fagron	L-proline	16J14-B01-327195	23109	40	20161116
Euro OTC	L-proline	1705021	23546	40	20170720*

Validation samples

A total of 280 317 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 *L-proline*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 8 reference samples from the substance/substance group *L-proline*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-proline	L1210046-02	21034	40
Euro OTC	L-proline	L1210046-02	21075	60
Euro OTC	L-proline	L1210046-01	21103	40
Fagron	L-proline	15D13-B02-308152	22270 [†]	20
Euro OTC	L-proline	1606010-01	23013	40
Euro OTC	L-proline	1606010-01	23100	40
Euro OTC	L-proline	1801047	23961	40
Euro OTC	L-proline	1812009	24419	40

- 126 572 spectra from a total of 2783 batches from further 781 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.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *L-proline*.

Supplier	Substance	Batch	Spectra
Euro OTC	L-proline	L1210046-03	1

- 78 928 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *L-proline* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-proline* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	248	72	126 572
Type C	0	1	0	78 928

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	77.5000 % (> 76.5625 %)
Type C	100.0000 % (> 99.8830 %)	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
22270	22270	0.00	60.81
23109	22270	3.36	63.23
23546	23546	0.00	45.02
22677	22677	0.00	56.01

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **L-serine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22289-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

L-serine; Serinum

Special notes

When selecting the *L-serine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *L-serine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	L-serine	1512012	22289	40	20160112*
Euro OTC	L-serine	1606020-01	22668	40	20160714
Euro OTC	L-serine	1711033	23914	40	20171208*

Validation samples

A total of 280 317 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 L-serine. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 L-serine.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-serine	1512012	22289 [†]	20
Euro OTC	L-serine	1606020	22678	40
Euro OTC	L-serine	1611006	22922	40
Euro OTC	L-serine	1809016	24296	40

- 126 752 spectra from a total of 2785 batches from further 781 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 1 batches from the substance/substance group L-serine.

*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	L-serine	1606020-01	3

- 78 926 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *L-serine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-serine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	130	10	126 752
Type C	0	3	0	78 926

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	92.8571 % (> 90.7143 %)
Type C	100.0000 % (> 99.8821 %)	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
22289	22289	0.00	67.51
22668	23914	5.07	59.28
23914	23914	0.00	63.02

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **L-threonine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20734-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

L-threonine; Threoninum

Special notes

When selecting the *L-threonine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *L-threonine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	L-threonine	12H02-N03	20734	40	1402580
Euro OTC	L-threonine	1210027-01	21033	40	1403152
Euro OTC	L-threonine	1601031	22378	40	20160225*

Validation samples

A total of 280 317 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 *L-threonine*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 [†].

- 260 spectra of 6 reference samples from the substance/substance group *L-threonine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-threonine	1210027-01	22319	60
Euro OTC	L-threonine	1606019	22679	40
Euro OTC	L-threonine	1609014	22792	40
Euro OTC	L-threonine	1703035	23158	40
Euro OTC	L-threonine	1711010	23738	40
Euro OTC	L-threonine	1811030	24417	40

- 126 632 spectra from a total of 2783 batches from further 781 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 *L-threonine*.

*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
Euro OTC	L-threonine	1606019-02	1
Fargon	L-threonine	2114720407	1

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *L-threonine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-threonine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	260	0	126 632
Type C	0	2	0	78 927

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.8823 %)	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
20734	20734	0.00	61.86
21033	21033	0.00	61.74
22378	22378	0.00	62.76

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **L-tryptophan**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20336-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

L-tryptophan; Tryptophanum

Special notes

When selecting the *L-tryptophan* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *L-tryptophan*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	L-tryptophan	14B05-B32-293485	21784	40	AR-15-FG-009473-01
Euro OTC	L-tryptophan	1506003	21866	40	20150630*
Euro OTC	L-tryptophan	1712006	23876	40	20180105*

Validation samples

A total of 280 317 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 L-tryptophan. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 [†].

- 260 spectra of 7 reference samples from the substance/substance group L-tryptophan.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	L-tryptophan	14B05-B32-293485	21784 [†]	20
Euro OTC	L-tryptophan	1506003	21866 [†]	20
Euro OTC	L-tryptophan	1506003	21871	60
Fagron	L-tryptophan	16E11-B03-322919	23195	40
Fagron	L-tryptophan	17G19-B01-343931	23998	40
Euro OTC	L-tryptophan	1806006	24144	40
Euro OTC	L-tryptophan	1812002	24426	40

- 126 632 spectra from a total of 2783 batches from further 781 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*.

- 10 spectra from 3 *Apo-Ident* customers from 5 batches from the substance/substance group *L-tryotophan*.

Supplier	Substance	Batch	Spectra
euroct/gehe	L-tryotophan	1212010-01	5
Euro OTC	L-tryotophan	1307004-01	2
Caelo	L-tryotophan	131046	1
Euro OTC	L-tryotophan	1506003-03	1
Euro OTC	L-tryotophan	1712006-01	1

- 78 919 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *L-tryotophan* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-tryotophan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	260	0	126 632
Type C	0	10	0	78 919

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.8818 %)	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
21784	21784	0.00	28.61
21866	21866	0.00	26.96
23876	23876	0.00	27.78

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Lysine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20385-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lysine hydrochloride; Lysine HCl; Lysini hydrochloridum

Special notes

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

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Lysine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Lysine hydrochlo...	15B09-B06-304170	21963	40	20150220
Fagron	Lysine hydrochlo...	14H20-B03-301894	21983	40	AR-16-FG-005856-01
Euro OTC	Lysine hydrochlo...	1708009	23698	40	20170922*

Validation samples

A total of 280317 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 *Lysine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 *Lysine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Lysine hydrochloride	12B14-N08	20735	40
Fagron	Lysine hydrochloride	15B09-B06-304170	21963 [†]	20
Fagron	Lysine hydrochloride	14H20-B03-301894	21983 [†]	20
Euro OTC	Lysine hydrochloride	1603011	22527	40
Euro OTC	Lysine hydrochloride	1611021	22865	40
Euro OTC	Lysine hydrochloride	1805030	24123	40

- 126692 spectra from a total of 2783 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Lysine hydrochloride*.

*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
Fagron	Lysine hydrochloride	14H20-B03-301894	1
Euro OTC	Lysine hydrochloride	1708009-01	2
Euro OTC	Lysine hydrochloride	1805030-01	1

- 78 925 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Lysine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lysine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	40	126 692
Type C	0	3	1	78 925

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	80.0000 % (> 78.5000 %)
Type C	100.0000 % (> 99.8820 %)	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
21963	21983	4.00	70.13
21983	21983	0.00	74.36
23698	23698	0.00	71.23

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Macrogols 1500**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20112-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Macrogols 1500; Macrogolum 1500

Special notes

When selecting the *Macrogols 1500* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

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

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

Finally, 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 *Macrogols 1500*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogols 1500	12324607	20977	40	1403323
Euro OTC	Macrogols 1500	1508002	21948	40	20150810*
Euro OTC	Macrogols 1500	1604005	22544	40	20160512*
Caelo	Macrogols 1500	17120001	23241	40	20170519
Caelo	Macrogols 1500	171200	23291	40	20170519*

Validation samples

A total of 280317 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 *Macrogols 1500*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 [†].

- 260 spectra of 7 reference samples from the substance/substance group *Macrogols 1500*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Macrogols 1500	1508002	21948 [†]	20
Euro OTC	Macrogols 1500	1705004	23423	40
Euro OTC	Macrogols 1500	1705036	23440	40
Caelo	Macrogols 1500	172221	23625	40
Euro OTC	Macrogols 1500	1711032	23898	40
Euro OTC	Macrogols 1500	1806015	24147	40
Caelo	Macrogols 1500	182290	24350	40

- 126632 spectra from a total of 2782 batches from further 781 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*.

- 47 spectra from 17 *Apo-Ident* customers from 24 batches from the substance/substance group *Macrogols 1500*.

Supplier	Substance	Batch	Spectra
Euro OTC	Macrogols 1500	1103017-02	4
Euro OTC	Macrogols 1500	1206005-01	5
Caelo	Macrogols 1500	10105901	1
Caelo	Macrogols 1500	12109409	1
Caelo	Macrogols 1500	11071309	1
Euro OTC	Macrogols 1500	1304023-01	7
Caelo	Macrogols 1500	13140901	1
Caelo	Macrogols 1500	13140906	1
Caelo	Macrogols 1500	13140902	2
ACM / Herba	Macrogols 1500	KN-0826/10	1
Phönix	Macrogols 1500	14072402	1
Gehe	Macrogols 1500	14072409	1
Caelo	Macrogols 1500	14072412	1
Euro OTC	Macrogols 1500	1406004-01	2
Caelo	Macrogols 1500	15120007	1
Euro OTC	Macrogols 1500	1503026-01	4
Caelo	Macrogols 1500	15413101	1
Caelo	Macrogols 1500	15413105	5
Caelo	Macrogols 1500	16138407	1
Caelo	Macrogols 1500	15413111	1
Krieger	Macrogols 1500	1712002	1
Caelo	Macrogols 1500	17120002	2
Caelo	Macrogols 1500	18129503	1
Caelo	Macrogols 1500	18129506	1

- 78 882 spectra from 565 *Apo-Ident* customers from a total of 26 113 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Macrogols 1500* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Macrogols 1500* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	240	20	126 632
Type C	0	45	2	78 882

The substance/substance group *Macrogols 1500* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	92.3077 % (> 91.1538 %)
Type C	100.0000 % (> 99.8817 %)	95.7447 % (> 89.3617 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20977	20977	0.00	34.47
23241	23291	5.56	33.42
23291	23291	0.00	32.78
21948	21948	0.00	51.43
22544	22544	0.00	55.02

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Macrogols 4000**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20690-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Macrogols 4000; Macrogolum 4000

Special notes

When selecting the *Macrogols 4000* substance/substance group, the following information is displayed to the user:

- Advice for the distinction from Macrogol 6000: Macrogol 4000 cannot be certainly distinct from Macrogol 6000, which is however currently not deliverable in Germany. Please decide, if an additional analysis seems reasonable.

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Macrogols 4000*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogols 4000	12074116	20690	40	1401164
Caelo	Macrogols 4000	12318019	20975	40	1403322
Caelo	Macrogols 4000	12361502	21065	40	20130107

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogols 4000	13356616	21357	40	20131107
Euro OTC	Macrogols 4000	1507004	21841	40	0000010550
Fagron	Macrogols 4000	15B13-B04-305461	21886	40	AR-16-FG-004020-01
Euro OTC	Macrogols 4000	1508031	21903	40	20150914*
Euro OTC	Macrogols 4000	1605012	22567	40	20160606*
Euro OTC	Macrogols 4000	1605025	22570	40	20160603*
Fagron	Macrogols 4000	16F10-B04-325645	23021	40	20160822
Euro OTC	Macrogols 4000	1702003	23174	40	20170301*
Euro OTC	Macrogols 4000	1711016	23902	40	20171214*

Validation samples

A total of 280317 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 *Macrogols 4000*. These samples are listed above in the [calibration samples](#) section.
- 74016 spectra from a total of 1611 batches from further 372 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 [†].

- 700 spectra of 19 reference samples from the substance/substance group *Macrogols 4000*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogols 4000	11172433	20692	40
Euro OTC	Macrogols 4000	1507004	21841 [†]	20
Fagron	Macrogols 4000	15B13-B04-305461	21886 [†]	20
Euro OTC	Macrogols 4000	1508031	21903 [†]	20
Euro OTC	Macrogols 4000	1609018	22791	40
Euro OTC	Macrogols 4000	1701007	22983	40
Caelo	Macrogols 4000	170686	23280	40
Caelo	Macrogols 4000	171190	23282	40
Euro OTC	Macrogols 4000	1705019	23433	40
Euro OTC	Macrogols 4000	1707026	23537	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	Macrogols 4000	172081	23657	40
Caelo	Macrogols 4000	173039	23825	40
Euro OTC	Macrogols 4000	1804001	24089	40
Euro OTC	Macrogols 4000	1803029	24094	40
Caelo	Macrogols 4000	181974	24227	40
Caelo	Macrogols 4000	182154	24229	40
Euro OTC	Macrogols 4000	1810003	24339	40
Caelo	Macrogols 4000	182448	24352	40
Caelo	Macrogols 4000	183153	24360	40

- 126 192 spectra from a total of 2770 batches from further 781 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.

- 555 spectra from 157 *Apo-Ident* customers from 263 batches from the substance/substance group *Macrogols 4000*.

Supplier	Substance	Batch	Spectra
Caelo	Macrogols 4000	12074116	3
Caelo	Macrogols 4000	12074109	3
Caelo	Macrogols 4000	1172404	1
Caelo	Macrogols 4000	11172303	1
EuRho	Macrogols 4000	1206009-01	1
Fagron	Macrogols 4000	12F29-N01	1
Caelo	Macrogols 4000	12149108	1
Fagron	Macrogols 4000	12F13-N01	2
Fagron	Macrogols 4000	12I20-n03	1
Caelo	Macrogols 4000	12149113	2
Caelo	Macrogols 4000	12074102	1
Noweda	Macrogols 4000	12361502	2
Caelo	Macrogols 4000	1010023-02	1
Caelo	Macrogols 4000	12361506	3
Caelo	Macrogols 4000	12361502	3
Fagron	Macrogols 4000	13B20-N01	2
Fagron	Macrogols 4000	12L10-N06	2
Fagron	Macrogols 4000	12F29-N01	2
Euro OTC	Macrogols 4000	1202040-02	2
Caelo	Macrogols 4000	12361513	3
Caelo	Macrogols 4000	12318011	1
Caelo	Macrogols 4000	12361512	2
Phoenix	Macrogols 4000	12258901	1
Noweda	Macrogols 4000	12361512	1
Phönix	Macrogols 4000	1202040-02	1
Fagron	Macrogols 4000	13A10-N01	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	Macrogols 4000	13136001	3
Caelo	Macrogols 4000	12318019	1
Noweda	Macrogols 4000	13136003	1
Caelo	Macrogols 4000	3940608	1
Caelo	Macrogols 4000	IntCh217002	1
Alliance Healthcare	Macrogols 4000	12361512	2
Fagron	Macrogols 4000	26082013A	1
Fagron	Macrogols 4000	13E22-N03	6
Fagron	Macrogols 4000	280913C	2
Caelo	Macrogols 4000	1316003	1
Fagron	Macrogols 4000	13F12-N09	1
Caelo	Macrogols 4000	13136003	3
Fagron	Macrogols 4000	16102013A	1
Fagron	Macrogols 4000	13B20N01	1
Caelo	Macrogols 4000	12318027	1
Caelo	Macrogols 4000	13136009	3
Caelo	Macrogols 4000	13136010	1
Caelo	Macrogols 4000	12361518	3
Caelo	Macrogols 4000	13136011	4
Fagron	Macrogols 4000	2122013a	1
Fagron	Macrogols 4000	2122013b	1
DIV GH	Macrogols 4000	13/12	1
Caelo	Macrogols 4000	13335106	1
Fagron	Macrogols 4000	13G19-N08	2
Fagron	Macrogols 4000	20122013C	1
Fagron	Macrogols 4000	17012014A	1
Facron	Macrogols 4000	7022014C	1
Caelo	Macrogols 4000	13356601	4
Fagron	Macrogols 4000	13F12N09	1
Bombastus	Macrogols 4000	13136016	1
Fagron	Macrogols 4000	1112M-02103	1
Caelo	Macrogols 4000	13356602	3
Caelo	Macrogols 4000	13356611	2
Fagron	Macrogols 4000	3032014B	1
Hedinger	Macrogols 4000	13G19-N08	1
Caelo	Macrogols 4000	13356609	1
Gutenberg-Apotheke	Macrogols 4000	13356609	1
Caelo	Macrogols 4000	13356617	6
Fagron	Macrogols 4000	14A03-B01-289602	3
Caelo	Macrogols 4000	12074114	1
Caelo	Macrogols 4000	13335107	1
Fagron	Macrogols 4000	13130-N03	1
Caelo	Macrogols 4000	13356621	1
Fagron	Macrogols 4000	160514a	1
Euro OTC	Macrogols 4000	1305020-02	4
Caelo	Macrogols 4000	13335102	1
Fagron	Macrogols 4000	13I17-N03	1
Fagron	Macrogols 4000	26052014A	1
Caelo	Macrogols 4000	13356616	1
Fagron	Macrogols 4000	28052014B	1
GEHE 06.05.2014	Macrogols 4000	13356608	2
ANZAG 15.05.2014	Macrogols 4000	13356616	1
Caelo	Macrogols 4000	14061705	5
Henry Lamotte	Macrogols 4000	1213test	1
Caelo	Macrogols 4000	123Test	1
Caelo	Macrogols 4000		1
Fagron	Macrogols 4000	123Test	1
Sanacorp	Macrogols 4000	14061707	1
Fagron	Macrogols 4000	290714c	1
Caelo	Macrogols 4000	14061707	4

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Supplier	Substance	Batch	Spectra
Fagron	Macrogols 4000	914I-02103	1
Caelo	Macrogols 4000	13335120	1
Fagron	Macrogols 4000	13I30-N03	1
Fagron	Macrogols 4000	14A03B01	1
Fagron	Macrogols 4000	18082014C	1
Fagron	Macrogols 4000	25082014A	1
Caelo	Macrogols 4000	14061708	9
Fagron	Macrogols 4000	15092014A	1
Caelo	Macrogols 4000	14180503	1
Fagron	Macrogols 4000	13L30-B31	1
Fagron	Macrogols 4000	20092014A	1
Fagron	Macrogols 4000	14A03-B01-289605	2
Fagron	Macrogols 4000	30092014B	1
Fagron	Macrogols 4000	13356608	1
Caelo	Macrogols 4000	1180513	1
Caelo	Macrogols 4000	1401708	1
Fagron	Macrogols 4000	14D14-B06	1
Caelo	Macrogols 4000	1234	1
Fagron	Macrogols 4000	22122014A	1
Euro OTC	Macrogols 4000	130502002	1
Caelo	Macrogols 4000	14180511	2
Fagron	Macrogols 4000	8012015A	1
Caelo	Macrogols 4000	14196007	1
Caelo	Macrogols 4000	14061713	1
Fagron	Macrogols 4000	14D14-B06-293453	2
Euro OTC	Macrogols 4000	1005011-01	1
Caelo	Macrogols 4000	14180524	1
Caelo	Macrogols 4000	14180508	2
Fagron	Macrogols 4000	2022015A	1
Caelo	Macrogols 4000	14180520	3
Caelo	Macrogols 4000	14180525	3
Fagron	Macrogols 4000	10022015A	1
Fagron	Macrogols 4000	10022015B	1
Euro OTC	Macrogols 4000	140701001	1
Fagron	Macrogols 4000	14G21-B04-296899	1
Fagron	Macrogols 4000	14J03-B07300840	1
Caelo	Macrogols 4000	14180522	1
Caelo	Macrogols 4000	14196013	1
Fagron	Macrogols 4000	14K03-B07-300522	2
Caelo	Macrogols 4000	14352607	2
Caelo	Macrogols 4000	14352606	2
Caelo	Macrogols 4000	14352608	1
Fagron	Macrogols 4000	14G15-B07-295632	1
Fagron	Macrogols 4000	505201C	1
Fagron	Macrogols 4000	14J03-B07-300840	1
Caelo	Macrogols 4000	14352611	2
Fagron	Macrogols 4000	3114I-02103	1
Fagron	Macrogols 4000	21052015A	1
Caesar & Loretz GmbH	Macrogols 4000	14180520	1
Caelo	Macrogols 4000	14352613	5
Fagron	Macrogols 4000	8062015B	1
Fagron	Macrogols 4000	8062015C	1
Caelo	Macrogols 4000	14180504	1
Caelo	Macrogols 4000	14352614	1
Fagron	Macrogols 4000	22062015A	1
Caelo	Macrogols 4000	14352618	1
Caelo	Macrogols 4000	23061505	1
Fagron	Macrogols 4000	14K03-b07-300522	1
ACM	Macrogols 4000	KNC0366J15	2
Fagron	Macrogols 4000	13G19-N14	1

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Supplier	Substance	Batch	Spectra
Caelo	Macrogols 4000	15159504	2
Caelo	Macrogols 4000	13081501	1
Caelo	Macrogols 4000	14196017	1
Caelo	Macrogols 4000	15159502	3
Caelo	Macrogols 4000	14J03-B07-304700	3
Caesar&Loretz GmbH/Anzag	Macrogols 4000	14196017	1
Caelo	Macrogols 4000	15159515	4
Fagron	Macrogols 4000	15b03-b08-304701	1
Gatt-Koller	Macrogols 4000	1420/04153415	1
Gehe	Macrogols 4000	14K03-B07-300522	1
Euro OTC	Macrogols 4000	15159515	1
Fagron	Macrogols 4000	15B13-B04-305461	3
Caelo	Macrogols 4000	15159516	1
Caelo	Macrogols 4000	15335003	6
Fagron	Macrogols 4000	15A08-B03-302762	3
Gatt-Koller	Macrogols 4000	2792/07153315	1
Caelo	Macrogols 4000	15335007	4
Caelo	Macrogols 4000	15225003	4
Fagron	Macrogols 4000	15A08B03302762	1
Caelo	Macrogols 4000	15335001	8
Caelo	Macrogols 4000	15406301	6
Caelo	Macrogols 4000	15159514	3
Caelo	Macrogols 4000	15335002	3
Caelo	Macrogols 4000	15225001	1
Caelo	Macrogols 4000	15406303	3
Fagron	Macrogols 4000	15H10-B04-314037	2
Fagron	Macrogols 4000	15H10-B04-31407	1
phönix	Macrogols 4000	15406302	1
phönix	Macrogols 4000	1535007	1
Caelo	Macrogols 4000	4123585	1
Fagron	Macrogols 4000	15A08-B03-302761	1
Phoenix	Macrogols 4000	16023905	1
Caelo	Macrogols 4000	15406302	2
Euro OTC	Macrogols 4000	1508031-01	1
Caelo	Macrogols 4000	16023905	4
Caelo	Macrogols 4000	16023904	4
Fagron	Macrogols 4000	15/29-B01-318038	2
Caelo	Macrogols 4000	15225013	1
Fagron	Macrogols 4000	2215I-02103	1
Caelo	Macrogols 4000	15376503	3
Caelo	Macrogols 4000	16023903	4
Rondell Apotheke	Macrogols 4000	16023905	1
Euro OTC	Macrogols 4000	1508031-02	1
Fagron	Macrogols 4000	15I29-B01-318038	1
Fagron	Macrogols 4000	16A20-B15-320652	6
phönix	Macrogols 4000	16023904	1
phönix	Macrogols 4000	1502031-02	1
Euro OTC	Macrogols 4000	1507004-01	1
Fagron	Macrogols 4000	16a20-b15-320652	8
Fagron	Macrogols 4000	15376510	1
Caelo	Macrogols 4000	16152001	11
Fagron	Macrogols 4000	16A20-B15-320060	1
Caelo	Macrogols 4000	15376515	1
Caelo	Macrogols 4000	16152003	4
Caelo	Macrogols 4000	160912M	1
Caelo	Macrogols 4000	161017M/15406304	1
phönix	Macrogols 4000	1605012-01	1
WE:Sanacorp 19.10.2016 ...	Macrogols 4000	15406301	2
Fagron	Macrogols 4000	16152002	1
Cealo/Gehe	Macrogols 4000	16023907	1

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Supplier	Substance	Batch	Spectra
Caelo	Macrogols 4000	161202M/16152004	1
Caelo	Macrogols 4000	39393137	1
Caelo	Macrogols 4000	16152002	1
Caelo	Macrogols 4000	16267311	6
Caelo	Macrogols 4000	16267305	7
Caelo	Macrogols 4000	170105M16152004	1
Caelo	Macrogols 4000	15376519	1
Caelo	Macrogols 4000	16267307	9
Henry Lamotte Oils GMBH	Macrogols 4000	16267308/170127M	1
Sanacorp	Macrogols 4000	15376520	1
Caelo	Macrogols 4000	16308902	9
Caelo	Macrogols 4000	16308904	7
Caelo	Macrogols 4000	16267308	3
Caelo	Macrogols 4000	16267308/170227M	1
Gatt-Koller	Macrogols 4000	4643/01170417	2
Caelo	Macrogols 4000	16308905	3
Gehe	Macrogols 4000	16267307	1
Caelo	Macrogols 4000	170324M/16267308	1
phönix	Macrogols 4000	1701007-01	3
Caelo	Macrogols 4000	5041701	1
Caelo	Macrogols 4000	1030517	1
Caelo	Macrogols 4000	170504M/16308906	1
Caelo	Macrogols 4000	170529M/16267308	1
Caelo	Macrogols 4000	170612M/17035603	1
Caelo	Macrogols 4000	16308907	7
Caelo	Macrogols 4000	1508031-02	1
Caelo	Macrogols 4000	17035603	1
Caelo	Macrogols 4000	17035604	3
Caelo	Macrogols 4000	1200617/16368105	1
Kehr	Macrogols 4000	16308907	1
VDL	Macrogols 4000	16308906	1
Caelo	Macrogols 4000	170710M/17035603	1
Finteler Apotheke	Macrogols 4000	16308907	1
Caelo	Macrogols 4000	170817M/17035603	1
Caelo	Macrogols 4000	17119001	2
Finteler Apotheke	Macrogols 4000	17035607	1
Caelo	Macrogols 4000	17035607	2
Caelo	Macrogols 4000	17035606	3
Caelo	Macrogols 4000	170928M/17119002	1
Caelo	Macrogols 4000	16308908	2
Anzag	Macrogols 4000	17068603	1
Caelo	Macrogols 4000	17208103	11
Caelo	Macrogols 4000	17119005	2
Caelo	Macrogols 4000	17068603	2
Caelo	Macrogols 4000	171103M/17119002	1
Caelo	Macrogols 4000	1131117/16358107	1
Caelo	Macrogols 4000	1260917/16358105	1
Caelo	Macrogols 4000	28111706	1
Caelo	Macrogols 4000	16358107/1111217	1
Caelo	Macrogols 4000	171211M/17119003	1
Caelo	Macrogols 4000	17208105	1
Sanacorp	Macrogols 4000	17208104	1
Phönix	Macrogols 4000	1707026-01	1
Caelo	Macrogols 4000	16358107	1
AHD	Macrogols 4000	17E02-B03-335507	3
AHD	Macrogols 4000	17E02-B03	1
AHD	Macrogols 4000	16K25-B02-330527	3
Caelo	Macrogols 4000	1720103	1
Caelo	Macrogols 4000	17303903	1
Caelo	Macrogols 4000	17303902	5

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Supplier	Substance	Batch	Spectra
Sanacorp	Macrogols 4000	17303901	1
Caelo	Macrogols 4000	30041803	1
Caelo	Macrogols 4000	17337902/1250418	1
Caelo	Macrogols 4000	17337902/2190218	1
AHD	Macrogols 4000	11H11-B05340782	1
Caelo	Macrogols 4000	17303901	3
Caelo	Macrogols 4000	17337902/1300518	1
Caelo	Macrogols 4000	18106101	2
Fagron	Macrogols 4000	1803029-01	2
Caelo	Macrogols 4000	9061805	1
Caelo	Macrogols 4000	18106104	1
Fiebig	Macrogols 4000	17035607	1
calo	Macrogols 4000	17303902	1
Caelo	Macrogols 4000	18106103	4
Fagron	Macrogols 4000	16K25-B02-330527	1
Caelo	Macrogols 4000	18106106	1
Caelo	Macrogols 4000	18106105	5
Fagron	Macrogols 4000	17K06-B05-345076	1
AHD	Macrogols 4000	17K06-B05-345076	1
Caelo	Macrogols 4000	18106109	2
Caelo	Macrogols 4000	190920	1
Caelo	Macrogols 4000	17337901	3
Caelo	Macrogols 4000	18215404	2
Caelo	Macrogols 4000	18244805	4
Nachtestung-Verlängerung	Macrogols 4000	17/17	1
Caelo	Macrogols 4000	17337906	1
Kehr	Macrogols 4000	18106105	1
Caelo	Macrogols 4000	18215403	1
Alliance	Macrogols 4000	18215403	1
Caelo	Macrogols 4000	18315303	2

- 78 374 spectra from 565 *Apo-Ident* customers from a total of 25 877 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Macrogols 4000* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Macrogols 4000* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 016
Type B	0	700	0	126 017
Type C	0	551	4	78 371

The substance/substance group *Macrogols 4000* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 99.1429 %)
Type C	100.0000 % (> 99.8821 %)	99.2793 % (> 98.7387 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20690	20690	0.00	49.37
21065	20690	7.62	51.60
21357	21886	2.98	46.47
23021	21886	5.30	47.05
22567	22567	0.00	44.54
21841	21841	0.00	37.50
23902	23902	0.00	54.49
20975	20975	0.00	45.85
21886	21886	0.00	42.75
21903	21903	0.00	53.13
22570	22570	0.00	49.70
23174	23174	0.00	55.67

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Magnesium citrate, anhydrous**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20616-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Magnesium citrate, anhydrous; Magnesii citras anhydricus

Special notes

When selecting the *Magnesium citrate, anhydrous* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Magnesium citrate, anhydrous*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Magnesium citrat...	1501031	21794	40	AR-15-FG-007845-01
Euro OTC	Magnesium citrat...	1506020	21829	40	0000010379
Euro OTC	Magnesium citrat...	1507019	21860	40	0000010617
Euro OTC	Magnesium citrat...	1511018	22225	40	20151130*
Euro OTC	Magnesium citrat...	1602028	22505	40	20160314*
Euro OTC	Magnesium citrat...	1706007	23549	40	20170720*

Validation samples

A total of 280317 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 *Magnesium citrate, anhydrous*. These samples are listed above in the [calibration samples](#) section.
- 74256 spectra from a total of 1617 batches from further 372 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 10 reference samples from the substance/substance group *Magnesium citrate, anhydrous*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Magnesium citrate, anhydrous	1501031	21794 [†]	20
Euro OTC	Magnesium citrate, anhydrous	1506020	21829 [†]	20
Euro OTC	Magnesium citrate, anhydrous	1507019	21860 [†]	20
Euro OTC	Magnesium citrate, anhydrous	1511018	22225 [†]	20
Euro OTC	Magnesium citrate, anhydrous	1607006	22673	40
Euro OTC	Magnesium citrate, anhydrous	1701018	22998	40
Euro OTC	Magnesium citrate, anhydrous	1711018	23895	40
Euro OTC	Magnesium citrate, anhydrous	1803033	24088	40
Euro OTC	Magnesium citrate, anhydrous	1808020	24202	40
Euro OTC	Magnesium citrate, anhydrous	1810026	24308	40

- 126572 spectra from a total of 2779 batches from further 781 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.

- 6 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Magnesium citrate, anhydrous*.

Supplier	Substance	Batch	Spectra
Euro OTC	Magnesium citrate, anhydrous	1602028-01	1
Euro OTC	Magnesium citrate, anhydrous	1706007-01	2
APOrtha Deutschland GmbH	Magnesium citrate, anhydrous	17000809/0	1
Arktis	Magnesium citrate, anhydrous	894P/2418	1
Euro OTC	Magnesium citrate, anhydrous	1808020-01	1

- 78 923 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Magnesium citrate, anhydrous* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium citrate, anhydrous* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	280	40	126 572
Type C	0	6	0	78 923

The substance/substance group *Magnesium citrate, anhydrous* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	87.5000 % (> 86.5625 %)
Type C	100.0000 % (> 99.9819 %)	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
22505	22505	0.00	27.02
22225	22225	0.00	32.55
21794	21794	0.00	32.64
21829	21829	0.00	28.07
23549	23549	0.00	29.48
21860	21860	0.00	23.96

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Magnesium hydrogen aspartate tetrahydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20812-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Magnesium hydrogen aspartate tetrahydrate; Magnesii asparticum tetrahydricum

Special notes

When selecting the *Magnesium hydrogen aspartate tetrahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Magnesium hydrogen aspartate tetrahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Magnesium hydrog...	1204014-01	20812	40	1404588
Euro OTC	Magnesium hydrog...	1306045-01	21749	40	20130708
Euro OTC	Magnesium hydrog...	1605031	22682	40	20160617*

Validation samples

A total of 280 317 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 *Magnesium hydrogen aspartate tetrahydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Magnesium hydrogen aspartate tetrahydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Magnesium hydrogen aspartate...	1306045-01	21749 [†]	20
Euro OTC	Magnesium hydrogen aspartate...	1707010	23552	40
Euro OTC	Magnesium hydrogen aspartate...	1707010	23608	40
Euro OTC	Magnesium hydrogen aspartate...	1806011	24156	40

- 126 752 spectra from a total of 2786 batches from further 781 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 *Magnesium hydrogen aspartate tetrahydrate*.

*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	Magnesium hydrogen aspartate...	1605031-01	1

- 78 928 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Magnesium hydrogen aspartate tetrahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium hydrogen aspartate tetrahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	140	0	126 752
Type C	0	1	0	78 928

The substance/substance group *Magnesium hydrogen aspartate tetrahydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.8830 %)	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
20812	20812	0.00	60.82
21749	20812	4.69	60.76
22682	22682	0.00	63.71

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Magnesium hydrogen citrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20016-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Magnesium hydrogen citrate; Magnesii hydrogenocitras hydricus; Magnesium hydrogen citrate, hydrated

Special notes

When selecting the *Magnesium hydrogen citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Magnesium hydrogen citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Magnesium hydrog...	13389102	21445	40	20131205
Euro OTC	Magnesium hydrog...	1507010	21873	40	20150713*
Euro OTC	Magnesium hydrog...	1510033	22233	40	20151117*
Euro OTC	Magnesium hydrog...	1601005	22296	40	20160119*
Euro OTC	Magnesium hydrog...	1701003	22992	40	20170124*
Caelo	Magnesium hydrog...	15415014	23240	40	20160105

Validation samples

A total of 280 317 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 *Magnesium hydrogen citrate*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 13 reference samples from the substance/substance group *Magnesium hydrogen citrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Magnesium hydrogen citrate	13389102	21445 [†]	20
Euro OTC	Magnesium hydrogen citrate	1507010	21873 [†]	20
Euro OTC	Magnesium hydrogen citrate	1510033	22233 [†]	20
Euro OTC	Magnesium hydrogen citrate	1601005	22296 [†]	20
Euro OTC	Magnesium hydrogen citrate	1604002	22509	40
Euro OTC	Magnesium hydrogen citrate	1608004	22796	40
Euro OTC	Magnesium hydrogen citrate	1701004	22991	40
Euro OTC	Magnesium hydrogen citrate	1705010	23380	40
Euro OTC	Magnesium hydrogen citrate	1705009	23382	40
Euro OTC	Magnesium hydrogen citrate	1710007	23771	40
Caelo	Magnesium hydrogen citrate	173531	23788	40
Euro OTC	Magnesium hydrogen citrate	1802026	24064	40
Euro OTC	Magnesium hydrogen citrate	1811038	24425	40

- 126 452 spectra from a total of 2776 batches from further 781 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.

- 450 spectra from 149 *Apo-Ident* customers from 160 batches from the substance/substance group *Magnesium hydrogen citrate*.

Supplier	Substance	Batch	Spectra
Eu Rho	Magnesium hydrogen citrate	110600401	1
Euro OTC	Magnesium hydrogen citrate	1110026-01	2
Caelo	Magnesium hydrogen citrate	11372902	1
Fagron	Magnesium hydrogen citrate	11H05-N07	1
Caelo	Magnesium hydrogen citrate	12175801	1
Caelo	Magnesium hydrogen citrate	12175807	3
Eu Rho	Magnesium hydrogen citrate	1202034-01	1
Caelo	Magnesium hydrogen citrate	12175802	2
Caelo	Magnesium hydrogen citrate	26101203	1
Euro OTC	Magnesium hydrogen citrate	1208006-01	3
Caelo	Magnesium hydrogen citrate	12175810	5
Fagron	Magnesium hydrogen citrate	12G10-N01	2
Caelo	Magnesium hydrogen citrate	12238002	2
Caelo	Magnesium hydrogen citrate	12238012	1
Caelo	Magnesium hydrogen citrate	11044103	2
Caelo	Magnesium hydrogen citrate	12238004	3
Noweda	Magnesium hydrogen citrate	10163306	1
Caelo	Magnesium hydrogen citrate	12368003	8
Caelo	Magnesium hydrogen citrate	121033-01	1
Euro OTC	Magnesium hydrogen citrate	1211033-01	4
Fagron	Magnesium hydrogen citrate	1056239	1
Caelo	Magnesium hydrogen citrate	12368005	1
Caelo	Magnesium hydrogen citrate	12368004	2
Caelo	Magnesium hydrogen citrate	11193104	1
Caelo	Magnesium hydrogen citrate	19061316	1
Caelo	Magnesium hydrogen citrate	12368011	7
Caelo	Magnesium hydrogen citrate	80446188	1
Caelo	Magnesium hydrogen citrate	2368011	1
Caelo	Magnesium hydrogen citrate	12368002	3
Phönix	Magnesium hydrogen citrate	1211033-01	2
Euro OTC	Magnesium hydrogen citrate	1211033-02	4
Caelo	Magnesium hydrogen citrate	6081301	1
Caelo	Magnesium hydrogen citrate	12368014	1
Caelo	Magnesium hydrogen citrate	12368017	2
Caelo	Magnesium hydrogen citrate	12368014	2
Caelo	Magnesium hydrogen citrate	13194601	4
Caelo	Magnesium hydrogen citrate	12091303	1
Caelo	Magnesium hydrogen citrate	13233906	8
Fagron	Magnesium hydrogen citrate	13D30-N07	2
Caelo	Magnesium hydrogen citrate	13194603	1
EuRho/Phönix	Magnesium hydrogen citrate	1202034-02	1
Caelo	Magnesium hydrogen citrate	13233901	9
Euro OTC	Magnesium hydrogen citrate	1306034-01	2
Caelo	Magnesium hydrogen citrate	11372901	1
Eu Rho	Magnesium hydrogen citrate	1306034-01	1
Caelo	Magnesium hydrogen citrate	13233904	5
Caelo	Magnesium hydrogen citrate	27111306	1

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Supplier	Substance	Batch	Spectra
Caelo	Magnesium hydrogen citrate	90396169	1
Caelo	Magnesium hydrogen citrate	13233905	1
Caelo	Magnesium hydrogen citrate	13233907	2
Euro OTC	Magnesium hydrogen citrate	1306034-02	2
Caelo	Magnesium hydrogen citrate	13233911	3
Caelo	Magnesium hydrogen citrate	133233907	1
Caelo	Magnesium hydrogen citrate	411052-2-P	1
Dr. Paul Lohmann	Magnesium hydrogen citrate	1079474	1
Dr. Paul Lohmann	Magnesium hydrogen citrate	1078434	1
Euro OTC	Magnesium hydrogen citrate	130603402	1
Caelo	Magnesium hydrogen citrate	11021401	1
Fagron	Magnesium hydrogen citrate	13B22-N03	1
Caelo	Magnesium hydrogen citrate	913M-01829	1
Caelo	Magnesium hydrogen citrate	13389103	7
Caelo	Magnesium hydrogen citrate	13233907	2
Euro OTC	Magnesium hydrogen citrate	1311003-01	7
Fagron	Magnesium hydrogen citrate	13K11-B02-288161	1
Caelo	Magnesium hydrogen citrate	13389106	2
Dr. Paul Lohmann	Magnesium hydrogen citrate	1077866	2
EuRho/Phönix	Magnesium hydrogen citrate	1311003-01	1
Euro OTC	Magnesium hydrogen citrate	2114M1829	1
Fagron	Magnesium hydrogen citrate		1
Caelo	Magnesium hydrogen citrate	11061403	1
	Magnesium hydrogen citrate	1311003-01	1
Caelo	Magnesium hydrogen citrate	17061401	1
Euro OTC	Magnesium hydrogen citrate	1311003-02	1
Caelo	Magnesium hydrogen citrate	13233913	6
Fagron	Magnesium hydrogen citrate	13K11-B02-288161	1
Caelo	Magnesium hydrogen citrate	13233910	5
Euro OTC	Magnesium hydrogen citrate	140402301	1
Euro OTC	Magnesium hydrogen citrate	1404023-01	5
Euro OTC	Magnesium hydrogen citrate	120800602	1
AHD	Magnesium hydrogen citrate	13389103	1
Caelo	Magnesium hydrogen citrate	13389111	4
Caelo	Magnesium hydrogen citrate	133389111	1
Phoenix 15.10.14	Magnesium hydrogen citrate	1311003-01	1
Alliance health	Magnesium hydrogen citrate	13389111	2
Euro OTC	Magnesium hydrogen citrate	1080144	1
Caelo	Magnesium hydrogen citrate	13389107	2
Euro OTC	Magnesium hydrogen citrate	1407048-01	3
Ichthyl/Phönix	Magnesium hydrogen citrate	14/12-B02-298854	1
Caelo	Magnesium hydrogen citrate	14I12-B02-298854	1
Caelo	Magnesium hydrogen citrate	14265503	6
Sanacaorp	Magnesium hydrogen citrate	13389108	1
Caelo	Magnesium hydrogen citrate	7011504	1
Caelo	Magnesium hydrogen citrate	1014E-01829	1
Caelo	Magnesium hydrogen citrate	14265511	1
Caelo	Magnesium hydrogen citrate	14265505	2
Euro OTC	Magnesium hydrogen citrate	140704801	1
Gehe Kassel	Magnesium hydrogen citrate	14/12-B02-298854	1
Caelo	Magnesium hydrogen citrate	14265504	5
Euro OTC	Magnesium hydrogen citrate	1407048-02	3
VDL;27.02.15	Magnesium hydrogen citrate	13389111	1
Fagron	Magnesium hydrogen citrate	14I12-B02	1
Caelo	Magnesium hydrogen citrate		1
Fagron	Magnesium hydrogen citrate	14I12-B02-298854	1
Fagron	Magnesium hydrogen citrate	14/12-B02-298854	1
Caelo	Magnesium hydrogen citrate	14265517	1
Caelo	Magnesium hydrogen citrate	14265513	2
Euro OTC	Magnesium hydrogen citrate	1085730	2

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Supplier	Substance	Batch	Spectra
Euro OTC	Magnesium hydrogen citrate	1501026-01	3
Caelo	Magnesium hydrogen citrate	14265514	1
ACM	Magnesium hydrogen citrate	KNC0829J15	1
Caelo	Magnesium hydrogen citrate	14265521	1
Nowed18.08.2015	Magnesium hydrogen citrate	14265521	1
Euro OTC	Magnesium hydrogen citrate	1507010-01	11
Caelo	Magnesium hydrogen citrate	14265516	2
Caelo	Magnesium hydrogen citrate	1214	1
Euro OTC	Magnesium hydrogen citrate	1507010-02	2
Caelo	Magnesium hydrogen citrate	15296702	3
Caelo	Magnesium hydrogen citrate	15296801	3
Heidelberger Chlorella/...	Magnesium hydrogen citrate	10032	1
Caelo	Magnesium hydrogen citrate	15296701	6
ACM	Magnesium hydrogen citrate	KNC1377J15	2
Caelo	Magnesium hydrogen citrate	315E-01829	1
Fagron	Magnesium hydrogen citrate	15296701	1
Euro OTC	Magnesium hydrogen citrate	151003301	1
Euro OTC	Magnesium hydrogen citrate	1510033-01	2
Euro OTC	Magnesium hydrogen citrate	160100501	1
Caelo	Magnesium hydrogen citrate	1601005-01	1
Euro OTC	Magnesium hydrogen citrate	1601005-01	10
Caelo	Magnesium hydrogen citrate	15296712	2
Euro OTC	Magnesium hydrogen citrate	1604002-01	31
Caelo	Magnesium hydrogen citrate	15296709	4
Caelo	Magnesium hydrogen citrate	15415001	4
Euro OTC	Magnesium hydrogen citrate	1604002-012x	1
phönix	Magnesium hydrogen citrate	1601005-01	2
phönix	Magnesium hydrogen citrate	15296702	1
phönix	Magnesium hydrogen citrate	1604002-01	1
Caelo	Magnesium hydrogen citrate	15415003	4
Caelo	Magnesium hydrogen citrate	15415004	2
Euro OTC	Magnesium hydrogen citrate	1604002-02	7
Caelo	Magnesium hydrogen citrate	15415002	1
phönix	Magnesium hydrogen citrate	15296710	1
Caelo	Magnesium hydrogen citrate	15415005	3
Caelo	Magnesium hydrogen citrate	15296710	1
Caelo	Magnesium hydrogen citrate	1604002-01	1
Phönix	Magnesium hydrogen citrate	15415005	1
Euro OTC	Magnesium hydrogen citrate		2
Caelo	Magnesium hydrogen citrate	16E02-B03-321485	1
Caelo	Magnesium hydrogen citrate	516Q-01829	1
Caelo	Magnesium hydrogen citrate	15415009	4
Euro OTC	Magnesium hydrogen citrate	1608004-01	20
Caelo	Magnesium hydrogen citrate	15415010	8
phönix	Magnesium hydrogen citrate	15415010	1
Euro OTC	Magnesium hydrogen citrate	1604002-001	1
Caelo	Magnesium hydrogen citrate	1415013	1
Caelo	Magnesium hydrogen citrate	15415013	2
phönix	Magnesium hydrogen citrate	15415015	2
Caelo	Magnesium hydrogen citrate	15415014	4
Euro OTC	Magnesium hydrogen citrate	160800401	1
Caelo	Magnesium hydrogen citrate	16341707	1
Fagron	Magnesium hydrogen citrate	16E02-B03-0326874	1
/Sanacorp	Magnesium hydrogen citrate	90170	1
Euro OTC	Magnesium hydrogen citrate	1701003-01	6
Euro OTC	Magnesium hydrogen citrate	1608004-02	2
Caelo	Magnesium hydrogen citrate	16341708	3
Caelo	Magnesium hydrogen citrate	16341709	2
phönix	Magnesium hydrogen citrate	16341709	2
Caelo	Magnesium hydrogen citrate	16341711	2

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Supplier	Substance	Batch	Spectra
phönix	Magnesium hydrogen citrate	1608004-01	1
Euro OTC	Magnesium hydrogen citrate	1705009-01	3
Caelo	Magnesium hydrogen citrate	16341710	4
Caelo	Magnesium hydrogen citrate	27101704	1
Euro OTC	Magnesium hydrogen citrate	1705010-01	4
Euro OTC	Magnesium hydrogen citrate	1701004-01	1
Noweda	Magnesium hydrogen citrate	16341710	1
Caelo	Magnesium hydrogen citrate	17173401	1
Caeolo/Gehe	Magnesium hydrogen citrate	17173405	2
Euro OTC	Magnesium hydrogen citrate	1710007-01	4
Anzag	Magnesium hydrogen citrate	16341710	1
Euro OTC	Magnesium hydrogen citrate	1710001-01	1
Fagron	Magnesium hydrogen citrate	17G24-B03-341019	1
Caelo	Magnesium hydrogen citrate	17173406	1
Caelo	Magnesium hydrogen citrate	1710007-01	1
lohmman	Magnesium hydrogen citrate	3054132	1
Euro OTC	Magnesium hydrogen citrate	1802026-01	2
Fiebig	Magnesium hydrogen citrate	1802026-01	1
Euro OTC	Magnesium hydrogen citrate	1808006-01	2
Fagron	Magnesium hydrogen citrate	3047166	1
Caelo	Magnesium hydrogen citrate	18216803	1
Kehr	Magnesium hydrogen citrate	17173406	1

- 78 479 spectra from 565 *Apo-Ident* customers from a total of 25 981 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Magnesium hydrogen citrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium hydrogen citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	440	0	126 452
Type C	0	437	13	78 479

The substance/substance group *Magnesium hydrogen citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.8817 %)	97.1111 % (> 96.4444 %)

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
21445	22233	2.83	33.96
23240	22992	2.60	36.68
21873	21873	0.00	35.08
22233	22233	0.00	34.17
22296	22296	0.00	35.20
22992	22992	0.00	37.25

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Magnesium orotate dihydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20429-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Magnesium orotate dihydrate; Magnesii oroticum dihydricum

Special notes

When selecting the *Magnesium orotate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Magnesium orotate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Magnesium orotat...	1511021	22287	40	20151228*
Caelo	Magnesium orotat...	162227	22638	40	20160809*
Caelo	Magnesium orotat...	16222701	23236	40	20160809
Euro OTC	Magnesium orotat...	1707018	23615	40	20170907*

Validation samples

A total of 280 317 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 *Magnesium orotate dihydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 [†].

- 260 spectra of 7 reference samples from the substance/substance group *Magnesium orotate dihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Magnesium orotate dihydrate	1511021	22287 [†]	20
Euro OTC	Magnesium orotate dihydrate	1608017	22784	40
Caelo	Magnesium orotate dihydrate	172157	23661	40
Caelo	Magnesium orotate dihydrate	172547	23799	40
Euro OTC	Magnesium orotate dihydrate	1712001	23874	40
Euro OTC	Magnesium orotate dihydrate	1802018	23963	40
Euro OTC	Magnesium orotate dihydrate	1808029	24200	40

- 126 632 spectra from a total of 2782 batches from further 781 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.

- 33 spectra from 16 *Apo-Ident* customers from 17 batches from the substance/substance group *Magnesium orotate dihydrate*.

Supplier	Substance	Batch	Spectra
Fagron	Magnesium orotate dihydrate	1000060461	1
Euro OTC	Magnesium orotate dihydrate	1209029-01	3
Euro OTC	Magnesium orotate dihydrate	1305011-01	1
Fagron	Magnesium orotate dihydrate	13H06-N07	1
Euro OTC	Magnesium orotate dihydrate	1305011-02	5
Fagron	Magnesium orotate dihydrate	12G05-N03	1
Euro OTC	Magnesium orotate dihydrate	130501102	1
Euro OTC	Magnesium orotate dihydrate	1407005-01	2
Fagron	Magnesium orotate dihydrate	14E20-B05-296005	1
Euro OTC	Magnesium orotate dihydrate	1504002-01	1
Fagron	Magnesium orotate dihydrate	14/13-B05-305616	1
Euro OTC	Magnesium orotate dihydrate	1511021-02	6
Caelo	Magnesium orotate dihydrate	14093607	2
Euro OTC	Magnesium orotate dihydrate	1608017-01	2
Euro OTC	Magnesium orotate dihydrate	1707018-01	2
Euro OTC	Magnesium orotate dihydrate	1712001-01	2
Euro OTC	Magnesium orotate dihydrate	1802018-01	1

- 78 896 spectra from 565 *Apo-Ident* customers from a total of 26 121 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Magnesium orotate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium orotate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	260	0	126 632
Type C	0	32	1	78 896

The substance/substance group *Magnesium orotate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.8817 %)	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
22287	22287	0.00	51.81
22638	22638	0.00	67.22
23236	22638	3.63	64.29
23615	23615	0.00	58.44

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Magnesium stearate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20707-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Magnesium stearate; Magnesii stearas

Special notes

When selecting the *Magnesium stearate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Magnesium stearate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Magnesium stearate	12C29-N06	20707	110	20120418
Fagron	Magnesium stearate	12D26-B03	21084	40	1407310
Caelo	Magnesium stearate	13095536	21117	40	20130405
Caelo	Magnesium stearate	14136929	21783	40	AR-15-FG-012028-01
Euro OTC	Magnesium stearate	1502033-01	22817	40	20150317

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 5 reference samples from the substance/substance group *Magnesium stearate*. These samples are listed above in the [calibration samples](#) section.
- 74226 spectra from a total of 1618 batches from further 372 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 6 reference samples from the substance/substance group *Magnesium stearate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Magnesium stearate	14136929	21783 [†]	20
Caelo	Magnesium stearate	162066	22763	40
Euro OTC	Magnesium stearate	1608022	22821	40
Euro OTC	Magnesium stearate	1704002	23436	40
Caelo	Magnesium stearate	181533	24215	40
Caelo	Magnesium stearate	183089	24354	40

- 126672 spectra from a total of 2783 batches from further 781 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.

- 17 spectra from 12 *Apo-Ident* customers from 14 batches from the substance/substance group *Magnesium stearate*.

[†]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	Magnesium stearate	12040307	1
Caelo	Magnesium stearate	13095536	1
Euro OTC	Magnesium stearate	1912I-01834	1
Fagron	Magnesium stearate	12D26-B03-289435	1
Caelo	Magnesium stearate	13095515	1
Euro OTC	Magnesium stearate	914I-01834	1
Caelo	Magnesium stearate	15155001	1
Euro OTC	Magnesium stearate	315E-01834	1
Caelo	Magnesium stearate	15305307	1
Caelo	Magnesium stearate	15305315	3
Caelo	Magnesium stearate	15305323	1
Caelo	Magnesium stearate	15305302	1
Caelo	Magnesium stearate	16206602	2
Euro OTC	Magnesium stearate	1116E-01834	1

- 78 912 spectra from 565 *Apo-Ident* customers from a total of 26 123 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Magnesium stearate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium stearate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 226
Type B	0	213	7	126 672
Type C	0	12	5	78 912

The substance/substance group *Magnesium stearate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9901 %)	96.8182 % (> 95.4545 %)
Type C	100.0000 % (> 99.8817 %)	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
20707	21084	14.56	45.63
21783	21783	0.00	27.39
22817	21783	3.75	32.56
21084	21084	0.00	48.76
21117	21084	23.87	82.13

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Manganese orotate dihydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22311-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Manganese orotate dihydrate

Special notes

When selecting the *Manganese orotate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Manganese orotate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Manganese orotat...	1601003	22311	40	20160113*
Euro OTC	Manganese orotat...	1801031	23908	40	20180131*

Validation samples

A total of 280317 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 *Manganese orotate dihydrate*. These samples are listed above in the [calibration samples](#) section.
- 74416 spectra from a total of 1621 batches from further 372 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 *Manganese orotate dihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Manganese orotate dihydrate	1601003	22311 [†]	20
Euro OTC	Manganese orotate dihydrate	1605029-01	22654	40
Euro OTC	Manganese orotate dihydrate	1605029-01	22737	40

- 126792 spectra from a total of 2787 batches from further 781 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 *Manganese orotate dihydrate*.

*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*.

- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Manganese orotate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Manganese orotate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	100	0	126 792
Type C	0	0	0	78 929

The substance/substance group *Manganese orotate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
22311	22311	0.00	54.81
23908	23908	0.00	49.13

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Mannitol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20118-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Mannitol; Mannitolum

Special notes

When selecting the *Mannitol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Mannitol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Mannitol	12305723	20980	40	1402329
Euro OTC	Mannitol	1508012	21884	40	20150827*
Euro OTC	Mannitol	1511025	22286	40	20151228*
Caelo	Mannitol	15197305	22581	40	20150720
Fagron	Mannitol	15A26-B01-305841	22883	40	20150204

Validation samples

A total of 280317 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 *Mannitol*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 [†].

- 890 spectra of 23 reference samples from the substance/substance group *Mannitol*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Mannitol	1508012	21884 [†]	20
Euro OTC	Mannitol	1511025	22286 [†]	20
Caelo	Mannitol	160140	22458	60
Euro OTC	Mannitol	1604008	22515	40
Caelo	Mannitol	16014013	22580	40
Caelo	Mannitol	162009	22614	40
Euro OTC	Mannitol	1606031	22697	40
Caelo	Mannitol	162121	22721	40
Euro OTC	Mannitol	1610027	22862	40
Fagron	Mannitol	15A26-B01-305841	22884	40
Caelo	Mannitol	162121	23066	30
Euro OTC	Mannitol	1703043	23125	40
Caelo	Mannitol	170879	23296	40
Caelo	Mannitol	160140	23299	40
Caelo	Mannitol	170879	23305	40
Caelo	Mannitol	170450	23318	40
Euro OTC	Mannitol	1708005	23700	40
Caelo	Mannitol	172588	23800	40
Euro OTC	Mannitol	1802004	23966	40
Euro OTC	Mannitol	1806024	24152	40
Euro OTC	Mannitol	1809008	24327	40
Caelo	Mannitol	182654	24368	40
Caelo	Mannitol	182655	24385	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.

- 126 002 spectra from a total of 2769 batches from further 781 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.

- 1143 spectra from 301 *Apo-Ident* customers from 327 batches from the substance/substance group *Mannitol*.

Supplier	Substance	Batch	Spectra
Euro OTC	Mannitol	1104028-03	3
Euro OTC	Mannitol	1110009-01	10
Gehe	Mannitol	12E24-N08	1
Caelo	Mannitol	1110009-02	1
Noweda	Mannitol	11219101	2
Euro OTC	Mannitol	1110009-02	4
Euro OTC	Mannitol	1104028-01	1
Euro OTC	Mannitol	1205016-01	11
Caelo	Mannitol	12105405	1
stumpf	Mannitol	1104028-02	1
Caelo	Mannitol	1205016-01	2
Noweda	Mannitol	11219138	1
Noweda	Mannitol	12105404	1
Caelo	Mannitol	12105420	7
Caelo	Mannitol	11219124	2
Caelo	Mannitol	12105403	3
Caelo	Mannitol	12105404	3
Fagron	Mannitol	11219122	1
EuRho	Mannitol	1911M-01844	1
Caelo	Mannitol	12105421	9
Caelo	Mannitol	11219122	1
Noweda	Mannitol	1205016-02	2
Caelo	Mannitol	11D01-N10	1
Fagron	Mannitol	11L19-N15	1
Caelo	Mannitol	20151012-2	1
Caelo	Mannitol	12105438	1
Euro OTC	Mannitol	12105433	3
Euro OTC	Mannitol	E671Z	1
Caelo	Mannitol	11219121	1
Caelo	Mannitol	9204719	1
Gehe/ Eurho	Mannitol	1205016-02	1
Caelo	Mannitol	10100026	2
Euro OTC	Mannitol	1205016-02	2
Caelo	Mannitol	5031304	1
Caelo	Mannitol	12305710	8
Caelo	Mannitol	1205016-02	2
Caelo	Mannitol	12305709	16
Caelo	Mannitol	12105433	5
EuRho	Mannitol	1205016-01	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
Euro OTC	Mannitol	1205016	1
Phönix	Mannitol	120501602	1
Euro OTC	Mannitol	1211034-01	9
Gehe	Mannitol	12J26-N15	1
Caelo	Mannitol	1211034-01	1
Caelo	Mannitol	11003611	1
Phagron	Mannitol	1302C004-279405	1
Phoenix	Mannitol	120501602	1
ANZAG	Mannitol	1211034-01	1
Klenk	Mannitol	1211034-02	2
Euro OTC	Mannitol	1211034-02	14
Fagron	Mannitol	12J26-N15	1
Phönix	Mannitol	12305723	1
Caelo	Mannitol	9081303	1
Phönix	Mannitol	1211034-02	1
Caelo	Mannitol	12305725	11
Fagron	Mannitol	12K28-N01	1
Caelo	Mannitol	23082013C	1
Fagron	Mannitol	1302C004	2
cesar&lorentz/Phönix	Mannitol	12305710	1
Caelo	Mannitol	12305724	5
Caelo	Mannitol	12305723	3
Euro OTC	Mannitol	1305043-01	12
Linden-Apotheke	Mannitol	1205016-02	1
Gehe	Mannitol	13E24-N01	1
Euro OTC	Mannitol	1305043	1
Caelo	Mannitol	12305726	1
Caelo	Mannitol	12305734	2
EuRho/Sanac	Mannitol	1305043-01	1
Caelo	Mannitol	24101306	1
EuRho	Mannitol	1211034-01	1
Euro OTC	Mannitol	130504301	1
Euro OTC	Mannitol	1006019-01	1
Phönix	Mannitol	1305043-01	1
Caelo	Mannitol	13189201	8
Caelo	Mannitol	12305725-3444311112	1
Caelo	Mannitol	11308807	2
Euro OTC	Mannitol	1305043-02	14
Caelo	Mannitol	12305740	2
Caelo	Mannitol	1230578	1
Caelo	Mannitol	13189203	8
gehe 10.12.13	Mannitol	1305043/01	1
Caelo	Mannitol	13189206	1
Caelo	Mannitol	16011402	1
Caelo	Mannitol	1305043-02	3
Noweda	Mannitol	1305043-01	1
Caelo	Mannitol	12305728	1
Euro OTC	Mannitol	1310004-01	14
Caelo	Mannitol	13189203-3566412081	1
Caelo	Mannitol	13189208	6
Caelo	Mannitol	13189215	17
GEHE	Mannitol	130504301	1
Euro OTC	Mannitol	17/14	1
Euro OTC	Mannitol	13189216	2
Caelo	Mannitol	13189207	7
Phoenix	Mannitol	1310004-01	1
Klenk	Mannitol	5224A110314	1
Gutenberg-Apotheke	Mannitol	1310004-01	4
Euro OTC	Mannitol	1310004-02	7
Hirsch	Mannitol	12305725	1

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Supplier	Substance	Batch	Spectra
Caelo	Mannitol	1310004-01	3
PHOENIX 24.04.2014	Mannitol	1310004-01	3
Fagron	Mannitol	1302C005	1
Gutenberg-Apotheke	Mannitol	13189221	1
Caelo	Mannitol	13189226	4
Gutenberg-Apotheke	Mannitol	1310004-02	1
Euro OTC	Mannitol	13155710	1
Caelo	Mannitol	16061401	1
Apomix	Mannitol	1310004-01	1
Sanacorp	Mannitol	1310004-01	1
Caelo	Mannitol	13189222	3
Sanacorp	Mannitol	13189215	1
Caelo	Mannitol	7071404	1
Caelo	Mannitol	14051204	8
Caelo	Mannitol	13189227	11
Fagron	Mannitol	13B01-B05-283812	1
Caelo	Mannitol	13095013	1
Anzag	Mannitol	1310004-02	1
Euro OTC	Mannitol	1404034-01	14
Caelo	Mannitol	12305736	4
Alliance Health 12.08.2...	Mannitol	1404034-01	2
Caelo	Mannitol	1404034-01	1
GEHE 24.07.2014	Mannitol	1310004-02	1
Caelo	Mannitol	14051207	1
Caelo	Mannitol	14051205	6
Fagron	Mannitol	13K20-B01-294194	2
EuRho	Mannitol	1404034-01	1
Euro OTC	Mannitol	1404034-02	15
Caelo	Mannitol	14051209	6
Caelo	Mannitol	2101401	1
EuRho	Mannitol	1404034-02	2
Caelo	Mannitol	13189228	1
Caelo	Mannitol	14051215	5
EuRhoPha	Mannitol	1404034-01	1
Caelo	Mannitol	14051208	2
Caelo	Mannitol	1400434-01	1
Caelo	Mannitol	4414E-01844	1
Caelo	Mannitol	13K20-B01-287704	1
Fagron	Mannitol	13E24N01	1
Euro OTC	Mannitol	10112014E	1
Caelo	Mannitol	1405127	1
Euro OTC	Mannitol	1409016-01	18
Beiersdorf	Mannitol	14051217	2
Caelo	Mannitol	14051224	2
Fagron	Mannitol	13K20-B01	1
Euro OTC	Mannitol	140403401	1
VDL;21.11.14;3,98EUR	Mannitol	13189227	1
Caelo	Mannitol	30121417	1
Caelo	Mannitol	10011501	1
Euro OTC	Mannitol	1409016-1	1
Caelo	Mannitol	14051223	1
Caelo	Mannitol	1409016-01	1
Fagron	Mannitol	13K20-B01-294193	1
Phönix	Mannitol	14051215	1
Euro OTC	Mannitol	14003402	1
Caelo	Mannitol	14051216	3
Caelo	Mannitol	14051230	2
Fagron	Mannitol	14G17-B06-301921	1
Caelo	Mannitol	14323101	3
Caelo	Mannitol	14051229	5

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Supplier	Substance	Batch	Spectra
Euro OTC	Mannitol	T03-07/1409016-01	1
Euro OTC	Mannitol	1409016-02	5
Fagron	Mannitol	12E24-N03	1
Fagron	Mannitol	14G04-B07	2
Caesar & Loretz GmbH	Mannitol	13189207	1
Caelo	Mannitol	30031502	1
xxxxx	Mannitol	xxxx	1
Caelo	Mannitol	14323103	2
Fagron	Mannitol	14G04-B07-296196	1
Caelo	Mannitol	14323105	2
Euro OTC	Mannitol	1502022-01	15
Noweda29.04.2015	Mannitol	14323113	1
Caelo	Mannitol	14323114	3
Fagron	Mannitol	1502022-01	3
Caelo	Mannitol	14323121	6
Caelo	Mannitol	14323113	1
Caelo	Mannitol	14323115	4
Fagron	Mannitol	13K20-B01-287698	2
Fagron	Mannitol	14G04-B07-301693	1
EuRho/GEHE	Mannitol	1409016-02	1
Euro OTC	Mannitol	15002022-01	1
EuRho/GEHE	Mannitol	1409016-01	1
Fagron	Mannitol	13K20-B01-292064	1
Allianz Healthcare 26.0...	Mannitol	1502022-01	1
Caelo	Mannitol	1502022-01	1
Caelo	Mannitol	15184101	1
Caelo	Mannitol	14323126	4
Fagron	Mannitol	14323121	1
Caelo	Mannitol	1423120	1
Caelo	Mannitol	14323120	1
Euro OTC	Mannitol	150202201	2
Caelo	Mannitol	14323127	3
Caelo	Mannitol	14323125	2
EuRho	Mannitol	1502022-02	1
Euro OTC	Mannitol	1502022-02	5
Caelo	Mannitol	14323129	1
Fagron	Mannitol	15B05-B04-304084	3
Fagron	Mannitol	14G04-B07-301694	1
Caelo	Mannitol	14323138	18
Fagron	Mannitol	720014-0002	1
Euro OTC	Mannitol	150202202	1
Caelo	Mannitol	14323124	2
Fagron	Mannitol	15A26-B01-304717	4
Euro OTC	Mannitol	1508012-01	20
EuRho	Mannitol	1508012-01	5
Noweda	Mannitol	14323124	1
Caelo	Mannitol	1508012-01	2
Gehe	Mannitol	1508012-01	1
Euro OTC	Mannitol	150801201	1
Caesar & Loretz GmbH	Mannitol	14323119	1
caelo/phoenix	Mannitol	14323138	2
Caelo	Mannitol	15197303	1
Caelo	Mannitol	15197301	12
Euro/Gehe	Mannitol	1508012-01	2
Noweda	Mannitol	15124-B05-314323	1
Caelo	Mannitol	15197302	5
Euro OTC	Mannitol	1502022/01	1
Noweda	Mannitol	15I24-B05-314323	1
Caelo	Mannitol	1508012-02	1
Euro OTC	Mannitol	158012-01	1

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Supplier	Substance	Batch	Spectra
Fagron	Mannitol	15K17-B01-315560	2
Cael Sanacorp 05.02.2016	Mannitol	14323138	2
Fagron	Mannitol	14G004-B07-301692	1
Euro OTC	Mannitol	1508012-02	10
Euro OTC	Mannitol	1511025-01	32
Fagron	Mannitol	14G04-B07-301692	10
Noweda	Mannitol	15K17-B01	1
Noweda	Mannitol	15B05-B06-304302	1
Euro OTC	Mannitol	140403402	1
WE:30.03.2016 Sanacorp	Mannitol	14323138	1
Fagron	Mannitol	15I24-B04	1
WE:16.03.2016 Sanacorp	Mannitol	14323124	1
Roquette Lestrem/Noweda	Mannitol	1508012-01	1
Euro OTC	Mannitol	151102501	2
Caelo	Mannitol	15197313	13
Fargon/ Noweda	Mannitol	15A26-B01-304717	1
phönix	Mannitol	14323138	1
Caelo	Mannitol	2274635	1
Euro OTC	Mannitol	151105-01	1
EuRho	Mannitol	1511025-01	1
Gehe/Euro	Mannitol	1511025-01	1
Caelo	Mannitol	48558	1
Defektur/eigen	Mannitol	1604008-01	1
Caelo	Mannitol	15K25-B04	1
Caelo	Mannitol	15525	1
Fagron	Mannitol	15K17-B03-314903	1
Phoenix	Mannitol	15197314	1
Caelo	Mannitol	15197314	4
Fagron	Mannitol	15K25-B04-317786	2
Euro OTC	Mannitol	1604008-01	27
Euro OTC	Mannitol	150801	1
Fagron	Mannitol	15K25-B06-318740	1
Caelo	Mannitol	1519713	1
Fagron	Mannitol	16D20-B03-320486	1
Fagron	Mannitol	16B24-B09-320013	2
Euro OTC	Mannitol	1511024-01	1
Phönix WE:02.08.2016 ...	Mannitol	15197313	1
Caelo	Mannitol	15197327	1
Caelo	Mannitol	15D28-B02-309192	4
EuRho/Phoenix	Mannitol	1508012-01	1
Euro OTC	Mannitol	16006031-01	1
Euro OTC	Mannitol	111100009-02	1
WE:Sanacorp 02.09.16 ...	Mannitol	16212101	1
Euro OTC	Mannitol	1604008	1
Caelo	Mannitol	16212103	1
Caelo	Mannitol	16212101	9
Caelo	Mannitol	1612101	1
Noweda	Mannitol	16D20-B04-320487	1
Caelo	Mannitol	16212102	8
Euro OTC	Mannitol	160408-01	1
Fagron	Mannitol	16D20-B03	1
Fagron	Mannitol	16212103	1
phönix	Mannitol	15197313	2
Euro OTC	Mannitol	150916M	1
Euro OTC	Mannitol	1604002-01	1
Fagron	Mannitol	16E11-B07-322830	2
Caelo	Mannitol	16014016	1
Fagron	Mannitol	16E11-B04	1
Caelo	Mannitol	16014014	1
Roquette Lestrem/Noweda	Mannitol	1511025-01	1

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Supplier	Substance	Batch	Spectra
WE:Sanacorp 25.10.2016 ...	Mannitol	16212102	2
Noweda	Mannitol	1508012-01	1
ALH	Mannitol	1409016-01	1
Euro OTC	Mannitol	160601-01	1
Caelo	Mannitol	160400801	1
Caelo	Mannitol	162121	1
Euro OTC	Mannitol	1606031-01	13
Euro OTC	Mannitol	161129M/1604008-01	1
Klenk	Mannitol	1606031-01	2
Celo	Mannitol	15197313	1
Fagron	Mannitol	16G27-B03-324517	1
Caelo	Mannitol	16212104	2
Fagron	Mannitol	16E11-B06	1
Fagron	Mannitol	16H02-B01-325660	1
Caelo	Mannitol	15197219	1
Euro OTC	Mannitol	160400	2
Gehe	Mannitol	15197313	1
Euro OTC	Mannitol	16040008-01	1
PHÖNIX	Mannitol	16212102	1
Fagron	Mannitol	16F27-B04-32483	1
Caelo	Mannitol	1621212	1
Caelo	Mannitol	16200904	2
Fagron	Mannitol	16F27-B05-324516	1
Caelo	Mannitol	15197329	1
allianz	Mannitol	16212101	2
Caelo	Mannitol	16014005	5
Caelo	Mannitol	16200909	1
Caelo	Mannitol	15197319	7
Caelo	Mannitol	16340301	12
Caelo	Mannitol	16200901	2
Caelo	Mannitol	16212109	3
Euro OTC	Mannitol	1606031-02	6
Caelo	Mannitol	8031704	1
Caelo	Mannitol	16340302	2
Fagron	Mannitol	16H29-B03-326641	1
Fagron	Mannitol	16H29-B05-327813	1
Euro OTC	Mannitol	1610027-01	22
Fagron	Mannitol	16E11B07322830	1
Fagron	Mannitol	16D20-B04-320487	1
Bombastus	Mannitol	16340301	1
Phoenix WE 10.03.17 EK...	Mannitol	16340302	1
Caelo	Mannitol	16212106	4
Fagron	Mannitol	16G27-B05-325659	1
Caesar	Mannitol	1508012-1	1
Caelo	Mannitol	16200903	7
Euro OTC	Mannitol	161002701	1
Caelo	Mannitol	16200908	2
Caelo	Mannitol	16014013	1
Fagron	Mannitol	13K20-B01-287706	1
Fagron	Mannitol	17A27-B02-331292	4
Fagron	Mannitol	17A27-B02	1
Caelo	Mannitol	1606031-02	1
Caelo	Mannitol	1610027-01	3
Euro OTC	Mannitol	160027-01	1
Caelo	Mannitol	16200916	2
Fagron	Mannitol	16L15-B04	1
Noweda	Mannitol	16L15-B05-329316	1
Euro OTC	Mannitol	16H29-B02	1
Fragron/Noweda	Mannitol	17A12-B04-330729	1
Fagron	Mannitol	16H25-B03-326639	1

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Supplier	Substance	Batch	Spectra
Caelo	Mannitol	16L15-B04-329317	1
Caelo	Mannitol	17045001	3
Fagron	Mannitol	16340301	1
Caelo	Mannitol	17045003	7
Noweda	Mannitol	P101P102P103	3
Caelo	Mannitol	16200913	1
Caelo	Mannitol	1071701	1
ApoIdent/Noweda	Mannitol	1610027-01	1
Euro OTC	Mannitol	1703043-01	9
Sanacorp	Mannitol	16200903	1
Caelo	Mannitol	16200912	1
Noewda	Mannitol	15197319	1
Caelo	Mannitol	1610018-01	1
Fagron	Mannitol	17A12-B02-332068	1
Caelo	Mannitol	163403	1
Fagron	Mannitol	16/28-B01-328593	1
Delta	Mannitol	1610027-01	1
Caelo	Mannitol	17045004	2
Fagron	Mannitol	17C28-B06	2
Caelo	Mannitol	16200924	3
Fagron	Mannitol	17B08-B02	1
Gehe	Mannitol	16200913	1
EuRho/Noweda	Mannitol	1703043-01	1
ALH	Mannitol	1703043-01	1
Caelo	Mannitol	170450	1
Caelo	Mannitol	16236603	1
Fagron	Mannitol	17D18-B03-335437	1
Fagron	Mannitol	17A12-Bo3	1
Caelo	Mannitol	17045002	10
Phönix	Mannitol	16200924	2
Euro OTC	Mannitol	170304301	1
Fagron	Mannitol	17C28-B05-33361	1
Caelo	Mannitol	151117	1
Sanacorp	Mannitol	16200924	1
Caelo	Mannitol	4516E-01844	1
Euro OTC	Mannitol	1703043-02	4
Fagron	Mannitol	17D12-B01-334435	1
Fagron	Mannitol	17D18-B01	1
Caelo	Mannitol	18121701	1
Euro OTC	Mannitol	1610027-02	1
Caelo	Mannitol	17087908	6
Fagron	Mannitol	17F27-B05-337913	1
Gehe	Mannitol	17F27-B05-337913	1
Caelo	Mannitol	17045006	2
Fagron	Mannitol	17045002	1
Caelo	Mannitol	17045009	5
Fagron	Mannitol	16L15-B04-329317	1
ceal	Mannitol	17045006	1
Euro OTC	Mannitol	1708005-01	12
Sanacorp E.K:19,49 -25...	Mannitol	17045009	1
Fagron	Mannitol	17/13-B04-340968	1
Fagron	Mannitol	17I13-B10	1
Euro OTC	Mannitol	180219M/1708005-01	1
Noweda	Mannitol	1708005-01	3
Apo Ident/ Noweda	Mannitol	1610027-01	1
Fagron	Mannitol	17I13-B11-341331	1
Caelo	Mannitol	17087916	5
Caelo	Mannitol	200218P302	1
Fagron	Mannitol	17I13-B04-340968	1
Caelo	Mannitol	17045010	3

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Supplier	Substance	Batch	Spectra
Caelo	Mannitol	17045008	5
Caelo	Mannitol	17087907	1
Euro OTC	Mannitol	17087908	1
Fagron	Mannitol	17/13-B11-341331	1
GEHE	Mannitol	17B08-B04-334312	1
Euro OTC	Mannitol	1708005-02	1
Fagron	Mannitol	17J30-B09-343413	2
Fagron	Mannitol	17J30-B10-343414	1
Fagron	Mannitol	720014-0001	1
Caelo	Mannitol	17J30-B10-3434414	1
Sanacorp	Mannitol	17087916	1
Fagron	Mannitol	17K29-B05	1
Caelo	Mannitol	17360101	3
Fagron	Mannitol	17J30309-343413	1
Caelo	Mannitol	9061808	1
Euro OTC	Mannitol	1802004-01	6
Caelo	Mannitol	E911K	1
Gehe	Mannitol	17L04-B03-345230	1
Euro OTC	Mannitol	170304302	1
ALH/EuRho	Mannitol	1802004-01	1
Caelo	Mannitol	17087915	1
Caelo	Mannitol	17258809	1
Euro OTC	Mannitol	E976E	1
Primavera/Phoenix	Mannitol	1708005-01	1
Caelo	Mannitol	17258808	1
Caelo	Mannitol	17360108	6
Caelo	Mannitol	1708005-01	1
Fagron	Mannitol	17J04-B06-341798	1
Sanacorp	Mannitol	17258809	1
Fagron	Mannitol	18A30-B08-346849	1
FragonFiebig	Mannitol	18A30-B07-348872	2
Caelo	Mannitol	17258812	2
Fagron	Mannitol	17A12-B02	1
Euro OTC	Mannitol	1806024-01	1
Caelo	Mannitol	27101802	1
Fagron	Mannitol	18B23-B10-349553	1
Fagron	Mannitol	18D09-B11-351436	2
Fagron	Mannitol	18D09-B13-352214	1
Sanacorp	Mannitol	17258808	1
Fagron	Mannitol	18E25-B07	1

- 77 786 spectra from 565 *Apo-Ident* customers from a total of 25 820 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Mannitol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mannitol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	876	14	125 922
Type C	0	1124	19	77 771

The substance/substance group *Mannitol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	98.4270 % (> 98.0899 %)
Type C	100.0000 % (> 99.8818 %)	98.3377 % (> 98.0752 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21884	21884	0.00	56.70
22286	22286	0.00	56.71
22581	22286	2.34	57.24
22883	22286	2.30	57.15
20980	20980	0.00	56.63

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Melatonin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20553-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Melatonin; Melatoninum

Special notes

When selecting the *Melatonin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Melatonin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Melatonin	12321404	20834	40	20121107
Caelo	Melatonin	12321411	20835	40	20121107
Caelo	Melatonin	12321415	20987	80	20121107
Euro OTC	Melatonin	1305029-02	21618	40	1411054
Euro OTC	Melatonin	1510041	22237	40	20151123*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Melatonin	15G06-B03-315183	22892	40	20150717
Fagron	Melatonin	15G06-B03-323733	22893	40	20150717
Euro OTC	Melatonin	1709020	23889	40	20180105*
Euro OTC	Melatonin	1804015	24128	40	20180522*
Euro OTC	Melatonin	1804015	24128SI	40	20180522*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Melatonin*. These samples are listed above in the [calibration samples](#) section.
- 74 056 spectra from a total of 1614 batches from further 372 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 [†].

- 379 spectra of 10 reference samples from the substance/substance group *Melatonin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Melatonin	1305029-02	21618 [†]	20
Euro OTC	Melatonin	1510041	22237 [†]	20
Euro OTC	Melatonin	1610040	22871	40
Caelo	Melatonin	163437	23036	40
Euro OTC	Melatonin	1811004	24330	40
Euro OTC	Melatonin	1510041	22237SI	60
Fagron	Melatonin	15G06-B03-315183	22892SI	40
Fagron	Melatonin	15G06-B03-323733	22893SI	40
Caelo	Melatonin	163437	23036SI	40
Euro OTC	Melatonin	1811004	24330SI	39

*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*.

- 126 513 spectra from a total of 2782 batches from further 781 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.

- 418 spectra from 136 *Apo-Ident* customers from 160 batches from the substance/substance group *Melatonin*.

Supplier	Substance	Batch	Spectra
Cealo/Gehe	Melatonin	10296624	1
Gehe	Melatonin	11/26-N07	1
Gehe	Melatonin	11L21-N04	1
Phönix	Melatonin	11267111	1
Euro OTC	Melatonin	1204003-02	12
Caelo	Melatonin	11267122	1
Caelo	Melatonin	1126109	1
Fagron	Melatonin	11F09-N02	1
Caelo	Melatonin	11267110	1
Caelo	Melatonin	11267121	1
Caelo	Melatonin	11267109	1
Caelo	Melatonin	11267119	1
Caelo	Melatonin	11267120	4
Gehe	Melatonin	12G19-N03	2
Caelo	Melatonin	20021312	1
Caelo	Melatonin	12321404	2
Euro OTC	Melatonin	12001	2
Fgron	Melatonin	12G19-N03	1
Caelo	Melatonin	12321406	1
Sanacorp	Melatonin	11267119	1
Caelo	Melatonin	2313M03554	1
Caelo	Melatonin	11267111	1
Caelo	Melatonin	11267102	1
Caelo	Melatonin	11267126	2
Caelo	Melatonin	10071303	1
Inresa	Melatonin	110005	1
Caelo	Melatonin	12321416	5
Caelo	Melatonin	12321411	1
Caelo	Melatonin	12321415	3
Fagron	Melatonin	12K13-N02	1
Fagron	Melatonin	12G19-N03	1
Caelo	Melatonin	13167301	8
Euro OTC	Melatonin	120400302	1
Fagron	Melatonin	13D12-N10	2
Fagron	Melatonin	13D12N10	1
Caelo	Melatonin	12321421	2
Gehe	Melatonin	13D12-N10	1
Caelo	Melatonin	120009	1
Caelo	Melatonin	16121303	1
Fagron	Melatonin	1305029-01	1
Fagron	Melatonin	13e22-n12	1
Gehe	Melatonin	13E22-N12	1
Phönix 02.01.2014	Melatonin	1204003-02	1
Anzag	Melatonin	12321415	1

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Supplier	Substance	Batch	Spectra
Caelo	Melatonin	12321422	4
Fagron	Melatonin	13E22N12	1
Fagron	Melatonin	120009	2
Euro OTC	Melatonin	120008	1
Fagron	Melatonin	13H21-N06	3
Euro OTC	Melatonin	1305029-01	8
Phönix 19.02.2014	Melatonin	13167301	2
GEHE 22.03.2014	Melatonin	13167302	1
KS Pharma	Melatonin	XPS130428	1
Phoenix 03.04.2014	Melatonin	12J19-N02	1
PHOENIX 14.04.2014	Melatonin	13E22-N12	1
Caelo	Melatonin	13167310	1
Fagron	Melatonin	13H21-N065x	1
Caelo	Melatonin	13167302	1
Cealo	Melatonin	12321422	1
Farmalabor / Farmalabor	Melatonin	P1201556-000	1
Caelo	Melatonin	13167309	1
Caelo	Melatonin	13167312	3
Fagron	Melatonin	13H29-B03-291180	2
Caelo	Melatonin	14110302	2
Caelo	Melatonin	1514E-03554	1
sanacorp	Melatonin	14110320	1
Fagron	Melatonin	14G18-B01-297245	1
Caelo	Melatonin	14110305	2
Fagron	Melatonin	13H29-B03	1
Caelo	Melatonin	14110308	3
Koisser	Melatonin	140202	2
Fagron	Melatonin	14G18-B01-297242	1
Phönix 02.01.15	Melatonin	13H21-N06	1
Caelo	Melatonin	20021505	1
Fagron	Melatonin	13E22-N12	1
Euro OTC	Melatonin	1407028-01	1
Caelo	Melatonin	13167314	5
Fagron	Melatonin	14G18-B01-297244	1
Caelo	Melatonin	15093001	6
Caelo	Melatonin	15093002	2
Caelo	Melatonin	14110316	1
Caelo	Melatonin	15093004	2
Euro OTC	Melatonin	1407028-02	2
Caelo	Melatonin	14110314	2
Caelo	Melatonin	15093010	5
Fagron	Melatonin	15C20-B01-308427	5
Caelo	Melatonin	15093008	8
Caelo	Melatonin	15254306	7
Caelo	Melatonin	15093013	2
Euro OTC	Melatonin	1510041-01	4
Caelo	Melatonin	15093012	2
Caelo	Melatonin	15254305	7
Caelo	Melatonin	15254308	6
Fagron	Melatonin	15C20-B01-306078	3
Caelo	Melatonin	15254307	10
Caelo	Melatonin	150601	1
Alliance	Melatonin	15254307	3
Alliance	Melatonin	15254316	1
Phoenix	Melatonin	15C20-B01	1
Caelo	Melatonin	15254313	2
Fagron	Melatonin	15C20-B01-308426	2
Fagron	Melatonin	15C20-B01-306077	1
Fagron	Melatonin	15G06-B03-315183	5
Caelo	Melatonin	1524309	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Melatonin	15254316	1
phönix	Melatonin	15254308	1
Caelo	Melatonin	15254319	6
Caelo	Melatonin	15254320	3
Caelo	Melatonin	15254321	5
Caelo	Melatonin	160125M	1
Caelo	Melatonin	15G06-B03-321299	1
Caelo	Melatonin	15254324	4
Caelo	Melatonin	15254336	4
Caelo	Melatonin	15254327	1
gepepharm	Melatonin	15G06-B03-315183	1
WE Sanacorp 28.11..2016...	Melatonin	15254324	1
Gehe	Melatonin	15254324	1
Fagron	Melatonin	15G06-B03-318398	1
Caelo	Melatonin	15254331	3
Caelo	Melatonin	15254328	2
Fargon GmbH & Co.KG	Melatonin	16G06-B01-324743	1
Caelo	Melatonin	15254333	1
allianz	Melatonin	15254324	1
Caelo	Melatonin	15254332	2
Fagron	Melatonin	15G06-B03-321299	2
Caelo	Melatonin	15254338	6
Caelo	Melatonin	15G06-B03-321298	2
Gehe	Melatonin	1510041-01	1
Caelo	Melatonin	16266901	7
Caelo	Melatonin	16266908	2
Sanacorp	Melatonin	161004001	1
Caelo	Melatonin	15254325	1
Fagron	Melatonin	15G06-B03-321298	2
Fagron	Melatonin	15G06-B03-323733	1
Fagron	Melatonin	15C20-B01-327131	1
Fagron	Melatonin	16G06-B01-327131	2
Euro OTC	Melatonin	1610040-02	5
Caelo	Melatonin	16266909	9
Caelo	Melatonin	16266904	2
Fagron	Melatonin	16G06-B01-324743	1
Sanacorp	Melatonin	161004002	1
Caelo	Melatonin	16266906	1
Caelo	Melatonin	16343710	7
Sanaorp	Melatonin	16343707	1
Caelo	Melatonin	16343707	2
Fagron	Melatonin	16G06-B01-329142	1
apo ident	Melatonin	1610040-02	1
Fagron	Melatonin	16343702	1
Caelo	Melatonin	16343709	4
Caelo	Melatonin	16343705	1
Sanacorp	Melatonin	APALC/MLT/161101M	1
Fagron	Melatonin	17C22-B01-337090	3
Caelo	Melatonin	16343708	7
Caelo	Melatonin	17305101	1
Caelo	Melatonin	16343713	5
Fagron	Melatonin	16343708	1
Farmalabor	Melatonin	P1800033-000	1
Phönix	Melatonin	APALC/MCT17030111	1
Caelo	Melatonin	17305102	7
Sanacorp	Melatonin		1
Caelo	Melatonin	17305101-20180206Ma1	1
Fagron	Melatonin	17C22-B01-337091	1
Euro OTC	Melatonin	1709020-01	8
Caelo	Melatonin	17305106	2

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Supplier	Substance	Batch	Spectra
Farmalabor	Melatonin	R1804925	1
Euro OTC	Melatonin	17305106	1
Sanacorp	Melatonin	APALC/MLT/170301M	2
Caelo	Melatonin	16343711	2
Caelo	Melatonin	17305105	4
Caelo	Melatonin	17305110	4
Caelo	Melatonin	163437/13	1
Sanacorp WE: 17.0518 EK...	Melatonin	1709020-01	1
Caelo	Melatonin	26051805	1
Fagron	Melatonin	17128-B04-344439	1
Caelo	Melatonin	17305113	2
Caesar & Lorenz GmbH	Melatonin	17305106	1
Sanacorp	Melatonin	MLT/SEP/170901	1
Fagron	Melatonin	17128-B04-344440	1
Euro OTC	Melatonin	1804015-01	2
Audor Pharma	Melatonin	ALC/MLT/170901	1
Caelo	Melatonin	17305116	1
Sanacorp	Melatonin	APMLT170901M	1
Caelo	Melatonin	17305114	3
Caelo	Melatonin	17305119	2
Caelo	Melatonin	17305122	3
Caelo	Melatonin	17305118	1
Caelo	Melatonin	17305104	1
Bombastus	Melatonin	18210304	1
Caelo	Melatonin	17350119	1
Caelo	Melatonin	18210306	2
Sanacorp	Melatonin	APALC/MLT/170901M	1
Caelo	Melatonin	17128-B04-345376	1

- 78 511 spectra from 565 *Apo-Ident* customers from a total of 25 977 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Melatonin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Melatonin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	440	0	74 056
Type B	0	379	0	126 513
Type C	0	398	20	78 511

The substance/substance group *Melatonin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.4169 %)
Type C	100.0000 % (> 99.8817 %)	95.2153 % (> 94.4976 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20834	22237	22.99	56.22
20835	22237	4.72	45.40
22237	22237	0.00	44.48
23889	23889	0.00	43.34
20987	22237	4.28	45.49
21618	21618	0.00	45.85
24128	24128	0.00	43.66
22892	22237	2.21	44.65
22893	22237	3.04	44.29

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Menthol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20036-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Menthol; Mentholum

Special notes

When selecting the *Menthol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Menthol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Menthol	13377404	21443	40	20131212
Euro OTC	Menthol	1403022-02	21601	30	20140408
Euro OTC	Menthol	1509045	21932	40	20151008*
Euro OTC	Menthol	1603024	22657	40	20160429*
Euro OTC	Menthol	1608012	22825	40	20160902*
Fagron	Menthol	16L20-T04-044769	23596	40	20170116

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 230 spectra of 6 reference samples from the substance/substance group *Menthol*. These samples are listed above in the [calibration samples](#) section.
- 74266 spectra from a total of 1617 batches from further 372 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 [†].

- 410 spectra of 11 reference samples from the substance/substance group *Menthol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Menthol	13377404	21443 [†]	20
Euro OTC	Menthol	1403022-02	21601 [†]	30
Euro OTC	Menthol	1509045	21932 [†]	20
Caelo	Menthol	160956	22452	60
Euro OTC	Menthol	1701014	23005	40
Caelo	Menthol	170927	23312	40
Euro OTC	Menthol	1705022	23427	40
Caelo	Menthol	170927	23645	40
Caelo	Menthol	171889	23668	40
Euro OTC	Menthol	1802003	23951	40
Caelo	Menthol	181522	24233	40

- 126482 spectra from a total of 2779 batches from further 781 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.

- 735 spectra from 342 *Apo-Ident* customers from 202 batches from the substance/substance group *Menthol*.

Supplier	Substance	Batch	Spectra
Fagron	Menthol	11C01-N01	1
Caesar & Loretz GmbH, 4...	Menthol	11202910	1
Caelo	Menthol	11202901	1
Euro OTC	Menthol	1204036-01	8
Euro OTC	Menthol	1111020-01	1
Caelo	Menthol	11202910	5
Fagron	Menthol	12Cos-N03	1
Finze	Menthol	9221710	1
Caesar & Loretz GmbH, 4...	Menthol	12020402	1
Caelo	Menthol	12020402	5
Fagron	Menthol	12D23-N06	4
Fagron	Menthol	12F01-N14	2
Caelo	Menthol	7111201	1
EuRho	Menthol	2910A-01855	1
Caelo	Menthol	1202041	1
Noweda	Menthol	1204036-01	1
Caelo	Menthol	10008029-02	1
Caelo	Menthol	20200712-2	1
Caelo	Menthol	1204036-01	1
Anzag	Menthol	12/19-N10	1
Sanacorp	Menthol	1204036-01	1
Fagron	Menthol	12G20-N02	3
Euro OTC	Menthol	120-4036-02	2
Caelo	Menthol	12020411	8
Gehe	Menthol	12020411	1
Fagron	Menthol	12I19-N10	2
Euro OTC	Menthol	1204036-02	3
Caesar/Noweda	Menthol	12020403	1
Gehe/ 27.10.12 EuRho	Menthol	11219216	1
Euro OTC	Menthol	120403602	1
Fagron	Menthol	1219-N10	1
Euro OTC	Menthol	696773	1
Fagron	Menthol	12/19-N10	1
Caelo	Menthol	12246205	8
Euro OTC	Menthol	1210017-01	4
Caesar & Loretz GmbH, 4...	Menthol	12020411	1
Phönix	Menthol	12246204	1
EuRho	Menthol	1204036-02	1
Euro OTC	Menthol	1008029-01	1
Caelo	Menthol	12246204	1
Caelo	Menthol	1/AD1	1
Caelo	Menthol	12020410	1
Caelo	Menthol	25051301	1
Caelo	Menthol	10157615	1
Euro OTC	Menthol	1210017-02	11
Euro OTC	Menthol	1310J-01855	1
Euro OTC	Menthol	1204036-1	1
Fagron	Menthol	11G19-N07	1
Euro OTC	Menthol	1105028-01	1
Fagron	Menthol	13D16-N09	7
Fagron	Menthol	12C05-N03	1
Frey*Lau GmbH	Menthol	1305010-01	1

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Supplier	Substance	Batch	Spectra
Caelo	Menthol	13103901	23
Caelo	Menthol	130501001	1
Caelo	Menthol	IntCh311052	1
Sanacorp	Menthol	1210017-01	1
Caelo	Menthol	750137	1
Euro OTC	Menthol	1305010-01	7
Fagron	Menthol	13016-N09	1
Caelo	Menthol	12246203	1
Euro OTC	Menthol	721123	1
Europharm	Menthol	130501-01	1
Caelo	Menthol	12246211	3
Caesar & Loretz GmbH, 4. ...	Menthol	13103901	1
AHD	Menthol	1305010-01	1
Gehe	Menthol	13D16-N09	1
Caelo	Menthol	72173258	1
Caelo	Menthol	13159105	19
Caelo	Menthol	1320260	2
Caelo	Menthol	13159104	4
Fagron	Menthol	13D16-N090631/1300	1
Fagron	Menthol	13G09-N090204/520	1
Sanacorp	Menthol	13103901	1
Caesar/Noweda	Menthol	12246211	1
Euro OTC	Menthol	PM14	1
Caelo	Menthol	314Q01855	1
Sanacorp	Menthol	1305010-01	1
Caelo	Menthol	687711	1
Caelo	Menthol	29121103	1
Caelo	Menthol	3912A-01855	1
Phoenix	Menthol	750137	1
Phönix	Menthol	13159105	1
Euro OTC	Menthol	1305010-02	5
Alliance Health 14.04..14	Menthol	1305010-02	1
Fagron	Menthol	13G09-N09	1
Phoenix 15.04.2014	Menthol	12246211	1
Caelo	Menthol	25041402	1
Caelo	Menthol	13159110	2
Caelo	Menthol	19051401	1
Fagron	Menthol	13J21-N04	2
Caelo	Menthol	13377404	15
Caelo	Menthol	13377402	3
Euro OTC	Menthol	130501002	1
Euro OTC	Menthol	807862	1
Euro OTC	Menthol	140302201	2
Euro OTC	Menthol	1002019-03	1
Euro OTC	Menthol	1403022-01	2
Caelo	Menthol	13377408	2
Caelo	Menthol	11091405	1
Caelo	Menthol	13377409	9
Euro OTC	Menthol	6102014B	1
Phoenix	Menthol	1403022-02	1
Caelo	Menthol	13377407	2
Euro OTC	Menthol	1403022-02	7
Euro OTC	Menthol	14030222-02	1
Caelo	Menthol	1410004-01	2
Euro OTC	Menthol	1410004-01	14
Caelo	Menthol	1403022-01	1
Caelo	Menthol	13377412	3
Caelo	Menthol	13377413	1
Euro OTC	Menthol	140322-01	1
Caelo	Menthol	814A-01855	1

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Supplier	Substance	Batch	Spectra
Caelo	Menthol	14183004	12
Euro OTC	Menthol	141000401	1
Caelo	Menthol	1403022-02	1
Gehe	Menthol	13377412	1
Sanacorp	Menthol	6/AKD3	1
Euro OTC	Menthol	1410004-02	7
Caelo	Menthol	14183012	3
Caelo	Menthol	14183008	3
Imhof	Menthol	15-5401	1
Caelo	Menthol	13103802	1
Fagron	Menthol	14H29-M02	9
Caelo	Menthol		2
Fagron	Menthol	14H29-M04	1
Andreas Imhof	Menthol	8052015	1
Caelo	Menthol	14183011	1
Caelo	Menthol	14183017	3
Caelo	Menthol	15076101	7
Euro OTC	Menthol	1502006-01	13
Caelo	Menthol	14183014	2
Caelo	Menthol	14183006	1
Caelo	Menthol	14183020	1
Caelo	Menthol	1410004-02	1
Euro OTC	Menthol	150200601	1
Fagron	Menthol	15076101	1
Euro OTC	Menthol	1502006-02	15
Caelo	Menthol	15076113	5
VDL; 9.23EUR; 28.09.15	Menthol	15076113	1
Phönix Gotha	Menthol	1410004-01	1
Caelo	Menthol	15076106	9
Euro OTC	Menthol	858607	1
Fagron	Menthol	778301	1
Caelo	Menthol	15076115	1
Caelo	Menthol	15076104	1
Euro OTC	Menthol	15020006-02	1
Caelo	Menthol	515M-01855	1
Fagron	Menthol	858607	1
Noweda	Menthol	1410004-01	1
Caelo	Menthol	15076112	10
Gehe	Menthol	1502006-02	1
EuRho	Menthol	1305010-01	1
Caesar&Loretz,Phönix	Menthol	15076106	1
Caelo	Menthol	1507601	1
Retest	Menthol	1305010-02	1
Caelo	Menthol	15076215	1
Fagron	Menthol	750137	1
Caelo	Menthol	15363805	7
Euro OTC	Menthol	1502006	1
Caelo	Menthol	15363804	8
Euro OTC	Menthol	1509045	2
Caesar/Noweda	Menthol	15076111	2
Frey+Lau GmbH	Menthol	1509045-02	1
Fagron	Menthol	1509045-03	1
Euro OTC	Menthol	1509045-03	8
Euro OTC	Menthol	1509045-02	8
Euro OTC	Menthol	1509045-01	2
Frey & Lau GmbH/Noweda	Menthol	1509045-03	2
Euro OTC	Menthol	150904502	1
Apo-ident	Menthol	1509045-03	1
EuRho	Menthol	915A-01855	1
Caelo	Menthol	15363803	2

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Supplier	Substance	Batch	Spectra
Caelo	Menthol	15076219	1
Euro OTC	Menthol	1603024-01	28
Caelo	Menthol	930716	1
Caelo	Menthol	1509045-03	1
Noweda	Menthol	15363809	1
Sanacorp WE:02.09.16 ...	Menthol	15363809	1
Caelo	Menthol	1603024-01	2
Caelo	Menthol	15363809	5
Caelo	Menthol	160719M	1
phönix	Menthol	15363805	1
Caelo	Menthol	15363810	6
Euro OTC	Menthol	1603021-01	1
Norex Flavours Pvt. Ltd. ...	Menthol	15286207	1
Norex Flavours Pvt. Ltd. ...	Menthol	15286205	2
WE:Sanacorp 03.11.2016 ...	Menthol	15363810	1
Caelo	Menthol	16095602	2
Gehe	Menthol	16095602	1
Caelo	Menthol	15286205	1
Caelo	Menthol	161202M/15076111	1
Caelo	Menthol	15363815	9
Caelo	Menthol	5315I-01855	1
Euro OTC	Menthol	1608012-01	15
Euro OTC	Menthol	1602024-01	1
Caelo	Menthol	16095606	11
Caelo	Menthol	16095603	3
Caesar & Loretz	Menthol	15363809	1
Ichthyol / Phoenix	Menthol	16095603	1
Euro OTC	Menthol	1608012-12	1
Caelo	Menthol	1536815	1
Euro OTC	Menthol	25021709	1
Caelo	Menthol	1608012-02	3
Caelo	Menthol	15286212	1
Caelo	Menthol	15286209	1
EuRho	Menthol	1603024-01	1
Euro OTC	Menthol	160801201	1
Caelo	Menthol	16095614	8
Euro OTC	Menthol	1608012-02	9
Euro OTC	Menthol	1701014-01	10
Euro OTC	Menthol	20116	1
Caelo	Menthol	15286216	1
Caelo	Menthol	16095604	1
Caelo	Menthol	16095613	11
Euro OTC	Menthol	1701014-02	12
Euro OTC	Menthol	170101402	2
Fagron	Menthol	1701014-02	1
Kehr	Menthol	16095613	1
Sanacorp	Menthol	16095613	1
Euro OTC	Menthol	16095614	1
Finteler Apotheke	Menthol	16095614	1
Sanacorp	Menthol	16095619	1
Caelo	Menthol	170822M/16095616	1
EuRho/Alliance	Menthol	1701014-01	1
Caelo	Menthol	16095616	1
Caelo	Menthol	16095619	6
Euro OTC	Menthol	1608012-1	1
Euro Ph. / Gehe	Menthol	1701014-02	1
Caelo	Menthol	17078004	1
Caelo	Menthol	15076118	1
beyvers	Menthol	16095613	1
Noweda	Menthol	1701014-02	1

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Supplier	Substance	Batch	Spectra
Eurho	Menthol	170502201	1
Gehe	Menthol	1705022-01	1
Caelo	Menthol	16095620	5
Cacolo/Gehe	Menthol	16096619	1
Caelo	Menthol	5117A-01855	1
Euro OTC	Menthol	18121718	1
Caelo	Menthol	160956	1
Caelo	Menthol	1705022-01	3
Euro OTC	Menthol	1705022-01	10
Caelo	Menthol	62470307	1
Euro OTC	Menthol	1705022	1
Caelo	Menthol	1701014-02	1
Fagron	Menthol	16L20T04044769	1
Anzag	Menthol	16L20-T04-044769	1
Euro OTC	Menthol	1701014-2	1
Euro OTC	Menthol	1001505	1
Caelo	Menthol	17188903	10
Caelo	Menthol	171889035483	1
Phoenix/Cealo	Menthol	1509045-01/4116F-018	1
Fagron	Menthol	16L20-T04-044769	5
Caelo	Menthol	17188906	2
Kehr	Menthol	16095620	1
Noweda	Menthol	17188904	1
Fagron	Menthol	16L20-To4	1
Caelo	Menthol	17188904	5
Euro OTC	Menthol	1802003-01	9
Euro OTC	Menthol	170502201	1
GEHE	Menthol	16L20-T04-044769	1
Caelo	Menthol	160956217188904	1
Caelo	Menthol	170502201	1
Fagron	Menthol	976035	1
Caelo	Menthol	16081805	1
Cealo	Menthol	1705022-01	1
Caelo	Menthol	19091805	1
Caelo	Menthol	1046973	1
Fagron	Menthol	16L20-T04-053177	1
Caelo	Menthol	16L20-T04-053177	1
Sanacorp	Menthol	17328804	1
Caelo	Menthol	17328804	4
Caelo	Menthol	1738804	1
Caelo	Menthol	1802003-01	1
Caelo	Menthol	17351505	1
Caelo	Menthol	18128007	1
Fagron	Menthol	1807044-01	1
Gehe	Menthol	1802003-01	1
Euro OTC	Menthol	16L20-T04-053177	1
Caelo	Menthol	18128009	2
Fagron	Menthol	18G02-T30-062159	1

- 78 194 spectra from 565 *Apo-Ident* customers from a total of 25 939 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Menthol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Menthol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	226	4	74 266
Type B	0	387	23	126 482
Type C	0	698	37	78 194

The substance/substance group *Menthol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	98.2609 % (> 96.9565 %)
Type B	100.0000 % (> 99.9901 %)	94.3902 % (> 93.6585 %)
Type C	100.0000 % (> 99.8817 %)	94.9660 % (> 94.5578 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21443	21932	2.42	79.45
21601	21932	2.69	79.60
21932	21932	0.00	79.05
23596	22825	2.22	81.61
22657	22657	0.00	78.62
22825	22825	0.00	81.99

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Mepivacaine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20710-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Mepivacaine hydrochloride; Mepivacaini hydrochloridum

Special notes

When selecting the *Mepivacaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Mepivacaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Mepivacaine hydr...	12A20-N12	20710	40	1401555
Fagron	Mepivacaine hydr...	13L04-B07-297077	21672	40	AR-15-FG-007876-01

Validation samples

A total of 280 317 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 *Mepivacaine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Mepivacaine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Mepivacaine hydrochloride	13L04-B07-297077	21672 [†]	20
Fagron	Mepivacaine hydrochloride	15I16-B01-322906	23212	40

- 126 832 spectra from a total of 2787 batches from further 781 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 5 batches from the substance/substance group *Mepivacaine hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	Mepivacaine hydrochloride	12F20-N07	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	Mepivacaine hydrochloride	13G05-N02	1
Fagron	Mepivacaine hydrochloride	13G05N02	1
Fagron	Mepivacaine hydrochloride	13G05-N02	1
Fagron	Mepivacaine hydrochloride	12E31-B40-305570	1
Fagron	Mepivacaine hydrochloride	15I16-B01	1

- 78 923 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Mepivacaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mepivacaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	60	0	126 832
Type C	0	5	1	78 923

The substance/substance group *Mepivacaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.8819 %)	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
20710	20710	0.00	33.03
21672	21672	0.00	32.40

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Mesalazine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21772-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Mesalazine; Mesalazinum

Special notes

When selecting the *Mesalazine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Mesalazine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Mesalazine	1206029-04	21772	40	AR-15-FG-011819-01
Euro OTC	Mesalazine	1206029-04	21887	40	20140923
Fagron	Mesalazine	15H13-B06-317177	22356	40	20150827
Euro OTC	Mesalazine	1602005	22518	40	20160218*
Euro OTC	Mesalazine	1602005-01	22925	40	20160218
Fagron	Mesalazine	16I28-B02-327679	22929	40	20161128

Validation samples

A total of 280 317 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 *Mesalazine*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1618 batches from further 372 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 5 reference samples from the substance/substance group *Mesalazine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Mesalazine	1206029-04	21772 [†]	20
Euro OTC	Mesalazine	1206029-04	21887 [†]	20
Fagron	Mesalazine	15H13-B06-317177	22356 [†]	20
Euro OTC	Mesalazine	1611019	22872	40
Fagron	Mesalazine	17A17-B03-336444	23934	40

- 126 752 spectra from a total of 2785 batches from further 781 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*.

- 30 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Mesalazine*.

Supplier	Substance	Batch	Spectra
Euro OTC	Mesalazine	1206029-04	1
Euro OTC	Mesalazine	1602005-01	2
Euro OTC	Mesalazine	1602005-02	3
Fagron	Mesalazine	16I28-B02-327679	24

- 78 899 spectra from 565 *Apo-Ident* customers from a total of 26 133 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Mesalazine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mesalazine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	140	0	126 752
Type C	0	27	3	78 899

The substance/substance group *Mesalazine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.8817 %)	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
22925	22518	1.36	49.08
22518	22518	0.00	48.50
21772	21772	0.00	39.78
21887	21772	7.61	40.38
22356	22518	3.06	46.55
22929	22518	5.28	45.00

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Metamizol sodium monohydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	22634-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metamizol sodium monohydrate; Metamizolum natricum monohydricum

Special notes

When selecting the *Metamizol sodium monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Metamizol sodium monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metamizol sodium...	161610	22634	40	20160714*
Caelo	Metamizol sodium...	15362816	22666	40	20151106

Validation samples

A total of 280317 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 *Metamizol sodium monohydrate*. These samples are listed above in the [calibration samples](#) section.
- 74416 spectra from a total of 1621 batches from further 372 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 *Metamizol sodium monohydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metamizol sodium monohydrate	15362815	22726	40
Caelo	Metamizol sodium monohydrate	161610	23313	40
Caelo	Metamizol sodium monohydrate	170584	23924	40

- 126772 spectra from a total of 2786 batches from further 781 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 *Metamizol sodium monohydrate*.

*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.

- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Metamizol sodium monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metamizol sodium monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	120	0	126 772
Type C	0	0	0	78 929

The substance/substance group *Metamizol sodium monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
22634	22634	0.00	48.88
22666	22634	7.17	48.86

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Methacholine chloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20733-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Methacholine chloride; Methacholinii chloridum

Special notes

When selecting the *Methacholine chloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Methacholine chloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Methacholine chl...	12F01-N04	20733	60	1403251
Caelo	Methacholine chl...	13260303	21251	40	20130827
Caelo	Methacholine chl...	13260303	21592	40	20130827
Caelo	Methacholine chl...	162293	22635	40	20160815*
Caelo	Methacholine chl...	16229304	22661	40	20160815

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Methacholine chl...	16229301	22662	40	20160815
Fagron	Methacholine chl...	16L20-B01-329966	22976	40	20170123
Fagron	Methacholine chl...	16L20-B01-329968	22977	40	20170123

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 340 spectra of 8 reference samples from the substance/substance group *Methacholine chloride*. These samples are listed above in the [calibration samples](#) section.
- 74 156 spectra from a total of 1616 batches from further 372 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 [†].

- 620 spectra of 14 reference samples from the substance/substance group *Methacholine chloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Methacholine chloride	13260302	21420	60
Caelo	Methacholine chloride	13260302	21590	60
Caelo	Methacholine chloride	13260303	21592 [†]	20
Caelo	Methacholine chloride	163299	23049	40
Caelo	Methacholine chloride	163299	23624	40
Fagron	Methacholine chloride	17H03-B02-346564	24287	40
Caelo	Methacholine chloride	13260302	21420SI	60
Caelo	Methacholine chloride	13260303	21592SI	60
Caelo	Methacholine chloride	162293	22635SI	40
Caelo	Methacholine chloride	16229304	22661SI	40
Caelo	Methacholine chloride	16229301	22662SI	40
Fagron	Methacholine chloride	16L20-B01-329966	22976SI	40
Fagron	Methacholine chloride	16L20-B01-329968	22977SI	40
Caelo	Methacholine chloride	163299	23049SI	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*.

- 126 272 spectra from a total of 2780 batches from further 781 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 12 *Apo-Ident* customers from 18 batches from the substance/substance group *Methacholine chloride*.

Supplier	Substance	Batch	Spectra
Fagron	Methacholine chloride	13/13-N03	2
Fagron	Methacholine chloride	13G10-N05	1
Fagron	Methacholine chloride	14G30-B03-296210	1
anzag 18.12.14 25,19	Methacholine chloride	14G30-B03-296209	1
Fagron	Methacholine chloride	10031504	1
Fagron	Methacholine chloride	24061503	1
	Methacholine chloride	14K20-B03-300973	2
Fagron	Methacholine chloride	312160	1
Fagron	Methacholine chloride	15F10-B02-315831	1
Fagron	Methacholine chloride	15F10-B02-315523	1
Fagron	Methacholine chloride	16L20-B01-329970	1
Fagron	Methacholine chloride	16L20-B01	1
Fagron	Methacholine chloride	17D13-B04	1
Fagron	Methacholine chloride	13121712	1
Phoenix/Cealo	Methacholine chloride	16L20-B01-329968	1
Fagron	Methacholine chloride	17D13-B04-334378	1
Caelo	Methacholine chloride	17D13-B04-334377	1
Fagron	Methacholine chloride	17H03-B02-346564	3

- 78 907 spectra from 565 *Apo-Ident* customers from a total of 26 119 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Methacholine chloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methacholine chloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	340	0	74 156
Type B	0	608	12	126 272
Type C	0	22	0	78 907

The substance/substance group *Methacholine chloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9901 %)	98.0645 % (> 97.5806 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 72.7273 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21592	20733	9.00	65.55
20733	20733	0.00	69.24
21251	20733	6.01	69.89
22661	20733	8.45	71.87
22976	20733	3.96	67.10
22977	20733	7.99	71.23
22635	22635	0.00	77.84
22662	22635	7.77	76.00

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Methionine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20971-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Methionine; Methioninum

Special notes

When selecting the *Methionine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Methionine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Methionine	12K01-N03	20971	40	1402432
Euro OTC	Methionine	L1404041-01	21751	40	20140508
Fagron	Methionine	13L19-B36-295115	21786	40	20140108
Euro OTC	Methionine	1602012	22368	40	20160219*
Caelo	Methionine	15404102	22727	40	AR-17-FG-000285-02
Caelo	Methionine	16274007	23258	40	20161014

Validation samples

A total of 280 317 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 *Methionine*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 6 reference samples from the substance/substance group *Methionine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Methionine	L1404041-01	21751 [†]	20
Fagron	Methionine	13L19-B36-295115	21786 [†]	20
Euro OTC	Methionine	1602012	22368 [†]	20
Euro OTC	Methionine	1609024	22787	40
Euro OTC	Methionine	1703042	23126	40
Euro OTC	Methionine	1710008	23777	40

- 126 712 spectra from a total of 2783 batches from further 781 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*.

- 4 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Methionine*.

Supplier	Substance	Batch	Spectra
Fagron	Methionine	13G09-N02	1
Fagron	Methionine	15A15-B08-307753	1
Euro OTC	Methionine	1602012-01	1
Caelo	Methionine	16274002	1

- 78 925 spectra from 565 *Apo-Ident* customers from a total of 26 133 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Methionine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methionine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	180	0	126 712
Type C	0	4	0	78 925

The substance/substance group *Methionine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8820 %)	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
22727	22727	0.00	51.98
23258	22727	4.36	51.45
20971	20971	0.00	70.78
21751	22368	3.39	68.85
21786	22368	4.49	69.84
22368	22368	0.00	67.59

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Methoxsalen**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20233-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Methoxsalen; Methoxsalenum

Special notes

When selecting the *Methoxsalen* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Methoxsalen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Methoxsalen	130604101	21555	40	20130805
Euro OTC	Methoxsalen	1506013	21862	40	20150706*
Euro OTC	Methoxsalen	1608019	22785	40	20160913*
Fagron	Methoxsalen	15J15-B03-321321	23165	40	20151124
Caelo	Methoxsalen	16103003	23167	40	20160415
Caelo	Methoxsalen	170781	23346	40	20170427*

Validation samples

A total of 280317 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 *Methoxsalen*. These samples are listed above in the [calibration samples](#) section.
- 74256 spectra from a total of 1617 batches from further 372 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 13 reference samples from the substance/substance group *Methoxsalen*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Methoxsalen	130604101	21555 [†]	20
Euro OTC	Methoxsalen	1506013	21862 [†]	20
Caelo	Methoxsalen	16103014	23166	40
Caelo	Methoxsalen	170781	23333	40
Euro OTC	Methoxsalen	1802021	24070	40
Euro OTC	Methoxsalen	130604101	21555SI	55
Euro OTC	Methoxsalen	1506013	21862SI	45
Euro OTC	Methoxsalen	1608019	22785SI	34
Fagron	Methoxsalen	15J15-B03-321321	23165SI	30
Caelo	Methoxsalen	16103014	23166SI	33
Caelo	Methoxsalen	16103003	23167SI	37
Caelo	Methoxsalen	170781	23333SI	40
Caelo	Methoxsalen	170781	23346SI	36

- 126422 spectra from a total of 2781 batches from further 781 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.

- 147 spectra from 69 *Apo-Ident* customers from 57 batches from the substance/substance group *Methoxsalen*.

Supplier	Substance	Batch	Spectra
Euro OTC	Methoxsalen	1104010-01	1
Fagron	Methoxsalen	11F21-N02	1
Noweda	Methoxsalen	11D07-N16	2
Fagron	Methoxsalen	11f21-n02	1
EuRho	Methoxsalen	1104010-01	1
Fagron	Methoxsalen	11D07-N16	1
Audor Pharma	Methoxsalen	AP1011024-01M	1
Fagron	Methoxsalen	12E02-N05	2
Euro OTC	Methoxsalen	1209015-01	3
Say Phytoceut. Ltd	Methoxsalen	1209015-01	3
Euro OTC	Methoxsalen	1203009-01	1
Fagron	Methoxsalen	2111A-03262	2
Nachprüfung	Methoxsalen	4211Q-03262	1
Euro OTC	Methoxsalen	120901501	1
Caelo	Methoxsalen	11376413	2
Fagron	Methoxsalen	12G02-N14	1
Fagron	Methoxsalen	MS01/13-14	1
Euro OTC	Methoxsalen	1306041-01	3
PHOENIX 18.02.14	Methoxsalen	1306041-01	2
Audor Pharma	Methoxsalen	1203009M	1
Fagron	Methoxsalen	14F06-B05-296501	2
Fagron	Methoxsalen	14f06-b05-296500	1
Phoenix	Methoxsalen	14F06-B05-296502	1
Fagron	Methoxsalen	14F06-B05-296500	1
Caelo	Methoxsalen	1409003-01	5
Caelo	Methoxsalen	1409003-02	1
Caelo	Methoxsalen	14F06-B05-296501	1
Euro OTC	Methoxsalen	140900302	1
Euro OTC	Methoxsalen	1409003-01	4
Caelo	Methoxsalen	11376433	1
Fagron	Methoxsalen	14F06-B05-301978	1
Euro OTC	Methoxsalen	1409003-02	2
Euro OTC	Methoxsalen	1503009-01	10
Caelo	Methoxsalen	1136428	1
Caelo	Methoxsalen	11376420	1
Caelo	Methoxsalen	1503009-01	2
Caelo	Methoxsalen	15099802	1
Herbal Creations/Caesar...	Methoxsalen	15244205	1
Phytoceut.Ltd	Methoxsalen	1503009-01	3
Herbal Creations/Caesar...	Methoxsalen	15244203	1
Euroo	Methoxsalen	1503009-01	1
Noweda	Methoxsalen	140900302	1
Fagron	Methoxsalen	15C10-B99-306266	1
Euro OTC	Methoxsalen	1503009-02	5
Euro OTC	Methoxsalen	1506013-01	12
Caelo	Methoxsalen	16/079/M	1
Caelo	Methoxsalen	15244204	3
Audor Pharma	Methoxsalen	AP15244213M	5
Fagron	Methoxsalen	15F23-B03-309644	1

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Supplier	Substance	Batch	Spectra
Caelo	Methoxsalen	15244209	1
Euro OTC	Methoxsalen	1506013-02	6
Herbal creations/Caesar...	Methoxsalen	15244208	1
Fagron	Methoxsalen	15F23-B03-318166	3
Herbal creations/Caesar...	Methoxsalen	15244212	1
Audor Pharma	Methoxsalen	15244213	1
Caelo	Methoxsalen	15244205	2
Audor Pharma	Methoxsalen	APHCFMPC16011M	6
Caelo	Methoxsalen	15244216	1
Fagron	Methoxsalen	15F23-B03	1
Euro OTC	Methoxsalen	1608019-01	2
Euro OTC	Methoxsalen	160801902	1
Fagron	Methoxsalen	15F23-B03-316262	1
Herbal Creations	Methoxsalen	1608019-01	1
Anzag	Methoxsalen	APHCFMPC16011M	1
Caelo	Methoxsalen	17078101	1
Euro OTC	Methoxsalen	1608019-02	4
Caelo	Methoxsalen	15244211	1
Caelo	Methoxsalen	17078108	1
Euro/Phönix	Methoxsalen	1608019-02	1
AHD	Methoxsalen	1608019-02	1
AHD	Methoxsalen	16103019	1
AHD	Methoxsalen	17078108	2
AHD	Methoxsalen	17078101	1
Euro OTC	Methoxsalen	1802021-01	2
Fagron	Methoxsalen	21111814	1

- 78 782 spectra from 565 *Apo-Ident* customers from a total of 26 080 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Methoxsalen* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methoxsalen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	384	86	126 422
Type C	0	147	0	78 782

The substance/substance group *Methoxsalen* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	81.7021 % (> 81.0638 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 95.9184 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21555	22785	6.31	78.16
21862	21862	0.00	78.70
22785	22785	0.00	78.15
23165	22785	6.35	75.92
23167	23346	6.19	75.49
23346	23346	0.00	74.87

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Methyl-4-hydroxybenzoate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20345-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Methyl-4-hydroxybenzoate; Methylis parahydroxybenzoas

Special notes

When selecting the *Methyl-4-hydroxybenzoate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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-4-hydroxybenzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Methyl-4-hydroxy...	11090034	20693	40	20110428
Euro OTC	Methyl-4-hydroxy...	1205025-01	20697	40	20120601
Euro OTC	Methyl-4-hydroxy...	1601037	22305	40	20160119*
Fagron	Methyl-4-hydroxy...	14L30-T01-018345	23223	40	20150309

Validation samples

A total of 280317 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 *Methyl-4-hydroxybenzoate*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 [†].

- 280 spectra of 7 reference samples from the substance/substance group *Methyl-4-hydroxybenzoate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Methyl-4-hydroxybenzoate	13268813	21439	60
Euro OTC	Methyl-4-hydroxybenzoate	1601037	22305 [†]	20
Caelo	Methyl-4-hydroxybenzoate	15063820	23216	40
Caelo	Methyl-4-hydroxybenzoate	171581	23317	40
Euro OTC	Methyl-4-hydroxybenzoate	1706005	23703	40
Euro OTC	Methyl-4-hydroxybenzoate	1807009	24148	40
Caelo	Methyl-4-hydroxybenzoate	181769	24223	40

- 126612 spectra from a total of 2782 batches from further 781 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*.

- 192 spectra from 140 *Apo-Ident* customers from 77 batches from the substance/substance group *Methyl-4-hydroxybenzoate*.

Supplier	Substance	Batch	Spectra
Caelo	Methyl-4-hydroxybenzoate	11090030	1
Caelo	Methyl-4-hydroxybenzoate	11090031	3
Gehe	Methyl-4-hydroxybenzoate	11090031	1
Gehe	Methyl-4-hydroxybenzoate	11090020	1
Caelo	Methyl-4-hydroxybenzoate	111003301	1
Eigenherstellung	Methyl-4-hydroxybenzoate	100912PML01	1
Caelo	Methyl-4-hydroxybenzoate	1108211930	1
Caelo	Methyl-4-hydroxybenzoate	11345115	7
Euro OTC	Methyl-4-hydroxybenzoate	172620	1
Anzag	Methyl-4-hydroxybenzoate	11345115	1
Fagron	Methyl-4-hydroxybenzoate	12H02-N08	1
Caelo	Methyl-4-hydroxybenzoate	9011303	1
Caelo	Methyl-4-hydroxybenzoate	11345120	2
Caelo	Methyl-4-hydroxybenzoate	713Q-01930	1
Caelo	Methyl-4-hydroxybenzoate	11345103	1
Fagron	Methyl-4-hydroxybenzoate	13B25-N03	2
Fagron	Methyl-4-hydroxybenzoate	20111125-1	1
Fagron	Methyl-4-hydroxybenzoate	13E27-N09	1
Caelo	Methyl-4-hydroxybenzoate	12251611	1
Caelo	Methyl-4-hydroxybenzoate	12251605	2
Fagron	Methyl-4-hydroxybenzoate	12D18-N01	1
Caelo	Methyl-4-hydroxybenzoate	12251624	5
Caelo	Methyl-4-hydroxybenzoate	12251619	1
Caelo	Methyl-4-hydroxybenzoate	13081308	1
AHD	Methyl-4-hydroxybenzoate	12251624	1
Caelo	Methyl-4-hydroxybenzoate	11090003	1
Euro OTC	Methyl-4-hydroxybenzoate	1009022-01	1
Euro OTC	Methyl-4-hydroxybenzoate	2606022	1
Fagron	Methyl-4-hydroxybenzoate		1
Caelo	Methyl-4-hydroxybenzoate	1251624	1
Phönix 14.01.2014	Methyl-4-hydroxybenzoate	12251624	1
phönix 4.12.2013	Methyl-4-hydroxybenzoate	1212011/01	1
Bombastus	Methyl-4-hydroxybenzoate	1212011-01	1
Caelo	Methyl-4-hydroxybenzoate	290114PML01	1
Caelo	Methyl-4-hydroxybenzoate	13268804	9
Caelo	Methyl-4-hydroxybenzoate	13268809	5
Caelo	Methyl-4-hydroxybenzoate	13268802	1
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	13268809	1
Caelo	Methyl-4-hydroxybenzoate	13268813	6
Caelo	Methyl-4-hydroxybenzoate	6091402	1
Euro OTC	Methyl-4-hydroxybenzoate	1401027-02	2
Caelo	Methyl-4-hydroxybenzoate	13268803	1
Euro OTC	Methyl-4-hydroxybenzoate	4312I-01930	1
Euro OTC	Methyl-4-hydroxybenzoate	1212011-01	1
GATT-KOLLER/PHOENIX	Methyl-4-hydroxybenzoate	6112/01142814	1
Caelo	Methyl-4-hydroxybenzoate	13268819	1
Caelo	Methyl-4-hydroxybenzoate	13268815	1
Phönix	Methyl-4-hydroxybenzoate	2AKD3	1
Caelo	Methyl-4-hydroxybenzoate	14120208	5
Euro OTC	Methyl-4-hydroxybenzoate	1502009-01	7
Euro OTC	Methyl-4-hydroxybenzoate	140600501	1
Euro OTC	Methyl-4-hydroxybenzoate	4314U-01930	1
Euro OTC	Methyl-4-hydroxybenzoate	1401027-01	1
Caesar&lorenz,Phoenix	Methyl-4-hydroxybenzoate	13268821	1
Caelo	Methyl-4-hydroxybenzoate	15063806	6

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Supplier	Substance	Batch	Spectra
Caelo	Methyl-4-hydroxybenzoate	12081502	1
Euro OTC	Methyl-4-hydroxybenzoate	1406005-01	1
Caelo	Methyl-4-hydroxybenzoate	15063802	6
Caelo	Methyl-4-hydroxybenzoate	15063803	1
Euro OTC	Methyl-4-hydroxybenzoate	1507042-01	10
Caelo	Methyl-4-hydroxybenzoate	13268821	1
Caelo	Methyl-4-hydroxybenzoate	15222203	3
EuRho	Methyl-4-hydroxybenzoate	110403101	1
Caelo	Methyl-4-hydroxybenzoate	15298102	12
Euro OTC	Methyl-4-hydroxybenzoate	1601037-01	4
Caesar/Noweda	Methyl-4-hydroxybenzoate	15063806	1
Caelo	Methyl-4-hydroxybenzoate	15298101	1
Caelo	Methyl-4-hydroxybenzoate	15063813	2
Euro OTC	Methyl-4-hydroxybenzoate	3115M-01930	1
Caelo	Methyl-4-hydroxybenzoate	15063818	2
Caelo	Methyl-4-hydroxybenzoate	1601037-01	4
Caelo	Methyl-4-hydroxybenzoate	15063819	4
PHÖNIX	Methyl-4-hydroxybenzoate	15063819	1
Caelo	Methyl-4-hydroxybenzoate	15063820	2
Caelo	Methyl-4-hydroxybenzoate	15444911	1
Caelo	Methyl-4-hydroxybenzoate	15063819/1210217	1
Caelo	Methyl-4-hydroxybenzoate	16256103	3
Euro OTC	Methyl-4-hydroxybenzoate	1507042-02	1
Caelo	Methyl-4-hydroxybenzoate	15444916	1
Caelo	Methyl-4-hydroxybenzoate	15444905	1
Fagron	Methyl-4-hydroxybenzoate	16256115	1
Caelo	Methyl-4-hydroxybenzoate	17158101	7
Caelo	Methyl-4-hydroxybenzoate	16256118	4
Caelo/Gehe	Methyl-4-hydroxybenzoate	16256104	1
Sanacorp E.K :2,76 - ...	Methyl-4-hydroxybenzoate	13268804	1
Caelo	Methyl-4-hydroxybenzoate	16256104	1
Gehe	Methyl-4-hydroxybenzoate	17158101	1
Caelo	Methyl-4-hydroxybenzoate	17343002	3
Noweda	Methyl-4-hydroxybenzoate	16256118	1
AHD	Methyl-4-hydroxybenzoate	17343002	1
Euro OTC	Methyl-4-hydroxybenzoate	1706005-01	1
Caelo	Methyl-4-hydroxybenzoate	17343013	1

- 78 737 spectra from 565 *Apo-Ident* customers from a total of 26 062 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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-4-hydroxybenzoate* can clearly be 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-4-hydroxybenzoate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	280	0	126 612
Type C	0	183	9	78 737

The substance/substance group *Methyl-4-hydroxybenzoate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.8817 %)	95.3125 % (> 93.7500 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20693	22305	7.83	62.14
20697	22305	7.62	61.97
22305	22305	0.00	61.57
23223	22305	8.65	60.35

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Methylcellulose**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20705-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Methylcellulose; Hypromellose 4000; Hypromellose E4M Prem; Methylcellulosum

Special notes

When selecting the *Methylcellulose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Methylcellulose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Methylcellulose	12D02-N09	20705	40	1402447
Caelo	Hypromellose 4000	13155006	20919	40	1402056
Caelo	Methylcellulose	13130115	21570	40	20130517
Caelo	Hypromellose 4000	14338801	21702	30	20141217
Caelo	Methylcellulose	160602	22457	40	20160323*
Fagron	Hypromellose 4000	15G08-B14-314845	22609	40	20150727

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 230 spectra of 6 reference samples from the substance/substance group *Methylcellulose*. These samples are listed above in the [calibration samples](#) section.
- 74 266 spectra from a total of 1617 batches from further 371 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 [†].

- 255 spectra of 8 reference samples from the substance/substance group *Methylcellulose*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hypromellose 4000	13155006	20931	40
Caelo	Methylcellulose	13130115	21570 [†]	20
Caelo	Hypromellose 4000	14338801	21702 [†]	15
Caelo	Methylcellulose	160602	22457 [†]	20
Caelo	Hypromellose 4000	162244	22757	40
Fagron	Methylcellulose	15H04-B07-331291	23224	40
Caelo	Hypromellose 4000	171150	23284	40
Caelo	Methylcellulose	171704	23627	40

- 126 637 spectra from a total of 2781 batches from further 780 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.

- 325 spectra from 183 *Apo-Ident* customers from 123 batches from the substance/substance group *Methylcellulose*.

Supplier	Substance	Batch	Spectra
Caelo	Methylcellulose	12044903	2
Caelo	Methylcellulose	10247604	1
Euro OTC	Methylcellulose	10247609	1
Caelo	Methylcellulose	12044907	1
Caelo	Methylcellulose	12044918	2
Caelo	Methylcellulose	12044917	1
Caelo	Methylcellulose	12044927	6
Caesar & Loretz GmbH	Methylcellulose	12044922	1
Caelo	Methylcellulose	13130104	5
Caelo	Methylcellulose	12044931	2
Caelo	Methylcellulose	12044922	2
Caelo	Methylcellulose	13130109	5
Caelo	Methylcellulose	13130115	5
Caelo	Methylcellulose	13021401	1
Caelo	Methylcellulose	20021401	1
Fagron	Methylcellulose	12H06-N06	2
Fagron	Methylcellulose	13E02-B03-290531	1
Caelo	Methylcellulose	13130121	3
Fagron	Methylcellulose	13/26-N04	1
Caelo	Methylcellulose	5081404	1
Fagron	Methylcellulose	131301(09)	1
Caelo	Methylcellulose	14197502	5
Caelo	Methylcellulose	14197514	7
Caelo	Methylcellulose	14197513	1
Caelo	Methylcellulose	15179602	11
Euro OTC	Methylcellulose	15179602	1
Fagron	Methylcellulose	15G08B14314845	1
Caelo	Methylcellulose	15179605	7
Caelo	Methylcellulose	16060206	11
Caelo	Methylcellulose	16060210	9
Caelo	Methylcellulose	16060202	1
Gehe	Methylcellulose	16284003	1
Caelo	Methylcellulose	16284003	2
Caelo	Methylcellulose	16284006	6
Caelo	Methylcellulose	1628404	1
Phoenix/Cealo	Methylcellulose	17170404	1
Caelo	Methylcellulose	16284004	1
Sanacorp	Methylcellulose	1717405	1
Caelo	Methylcellulose	17170405	2
Caelo	Methylcellulose	18045101	2
Bombastus	Methylcellulose	17170405	1
Fagron	Hypromellose 4000	12A30-N02	3
Caelo	Hypromellose 4000	12098702	1
Fagron	Hypromellose 4000	20110612-2	1
Caelo	Hypromellose 4000	12215504	2
Fagron	Hypromellose 4000	10G09-N03	1
Gehe / 26.10.12 Fragon	Hypromellose 4000	9D30-N05	1
Fagron	Hypromellose 4000	12E02-N03	3
Fagron	Hypromellose 4000	12G23-N03	1
Caelo	Hypromellose 4000	13100304	2
Fagron	Hypromellose 4000	ZH19012N12	1
Caelo	Hypromellose 4000	13155004	10
Fagron	Hypromellose 4000	12G23-N03	1
Fagron	Hypromellose 4000	12H20-N05	1

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Supplier	Substance	Batch	Spectra
Caelo	Hypromellose 4000	13d03-n03	1
Caelo	Hypromellose 4000	13155002	1
Fagron	Hypromellose 4000	13D03-N03	7
Fagron	Hypromellose 4000	1A01012N11	1
Fagron	Hypromellose 4000	13h09-m04	1
Fagron	Hypromellose 4000	12D03-N03	1
Fagron	Hypromellose 4000	YI16012N11	1
Alliance Health 27.12.2...	Hypromellose 4000	13D03-N03	1
Fagron	Hypromellose 4000	13D03N03	1
Fagron	Hypromellose 4000	13H09-N04	9
Fagron	Hypromellose 4000	1J31012N11	3
Noweda	Hypromellose 4000	1315505	1
Phonix	Hypromellose 4000	13H09-N04	1
Fagron	Hypromellose 4000	13E02-B03-290531	2
Phoenix	Hypromellose 4000	13E02-B03	1
Fagron	Hypromellose 4000	1K01012N11	1
Gatt-Koller / Phoenix	Hypromellose 4000	14C05-B03-291647	2
Fagron	Hypromellose 4000	13E02-B03-290532	1
Fagron	Hypromellose 4000	2H12012N12	1
Phoenix	Hypromellose 4000	14c05-b03-294708	1
Fagron	Hypromellose 4000	14C05-B03	1
Caelo	Hypromellose 4000	12239502	1
Fagron	Hypromellose 4000	14C05-B03-294708	4
Fagron	Hypromellose 4000	700182-0001	2
Fagron	Hypromellose 4000	14C05-B03-294711	1
Caelo	Hypromellose 4000	14338801	3
Fagron	Hypromellose 4000	14G02-B11-296851	1
Fagron	Hypromellose 4000	14c05-B03-294708	1
Caelo	Hypromellose 4000	14C05-B03-294708	1
DOW Chemical Company Mi...	Hypromellose 4000	14G02-B11-296850	1
Fagron	Hypromellose 4000	14C05B03	1
Phönix Gotha	Hypromellose 4000	14G02-B11-296850	1
Fagron	Hypromellose 4000	14G02-B11-296850	5
Fagron	Hypromellose 4000	14G02-B11-302118	5
Caelo	Hypromellose 4000	14338802	1
Fagron	Hypromellose 4000	14G02-B11	3
Fagron	Hypromellose 4000	14G02-B11-302121	1
Nachprüfung 2609	Hypromellose 4000	11H26-N01	1
Fagron	Hypromellose 4000	14G02-B11-302119	1
Fagron	Hypromellose 4000	15B02-B05	1
Fagron	Hypromellose 4000	14g02-b11-302118	2
Caelo	Hypromellose 4000	15B02-B05-308852	1
Fagron	Hypromellose 4000	15G08-B14-310845	7
Fagron	Hypromellose 4000	15g08-b14-310845	2
Fagron	Hypromellose 4000	15B02-B05-308852	1
Fagron	Hypromellose 4000	3G08012N11	1
Fagron	Hypromellose 4000	15G08B14314185	2
Fagron	Hypromellose 4000	15g08-b14-314845	1
Gehe	Hypromellose 4000	14G02-B11	1
Fagron	Hypromellose 4000	15G08-B14-314845	5
Fagron	Hypromellose 4000	15G08-B14	1
Fagron	Hypromellose 4000	16B16-B07-318276	1
Fagron	Hypromellose 4000	D180F8Q011	1
Fagron	Hypromellose 4000	16B16-B07-318531	6
FRAGON/Poenix	Hypromellose 4000	16B16-B07-18276	1
Fagron	Hypromellose 4000	16B16-B07-321327	2
Fagron	Hypromellose 4000	16B-16-B07-321327	1
Caelo	Hypromellose 4000	D180F8Q011	1
Jenne	Hypromellose 4000	15G08-B14	1
Caelo	Hypromellose 4000	15G08-B14-314845	3

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Supplier	Substance	Batch	Spectra
Fagron	Hypromellose 4000	16B16-B07-321579	1
Caelo	Hypromellose 4000	16224401	6
Phoenix	Hypromellose 4000	16B16-B07	1
Caelo	Hypromellose 4000	16224403	11
Fagron	Hypromellose 4000	16B16-B07-321328	1
Phönix	Hypromellose 4000	16224403	1
Caelo	Hypromellose 4000	16B16-B07-321327	2
Fagron	Hypromellose 4000	16B16B07	1
Fagron	Hypromellose 4000	16B16-B07-323114	3
Caelo	Hypromellose 4000	16224406	2
Caelo	Hypromellose 4000	16224407	4
Fagron	Hypromellose 4000	16H23-B02-332066	4
Caelo	Hypromellose 4000	16224409	3
Caelo	Hypromellose 4000	16224404	1
Caelo	Hypromellose 4000	17115005	5
Fagron	Hypromellose 4000	16B16-B07-325280	1
Caelo	Hypromellose 4000	180215H/17115004	1
Caelo	Hypromellose 4000	17115008	1
Caelo	Hypromellose 4000	171150085501	1
Kehr	Hypromellose 4000	17115005	1
Caelo	Hypromellose 4000	18132101	4
Fagron	Hypromellose 4000	17115005	1
Caelo	Hypromellose 4000	18132102	1
Cealo/Gehe	Hypromellose 4000	18132101	1
Caelo	Hypromellose 4000	18132105	4
Caelo	Hypromellose 4000	5121818	1
Fagron	Hypromellose 4000	18D04-B03	1
Fagron	Hypromellose 4000	18D04-B03-350745	1

- 78 604 spectra from 565 *Apo-Ident* customers from a total of 26 015 batches from a further 692 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Methylcellulose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methylcellulose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	230	0	74 266
Type B	0	255	0	126 637
Type C	0	316	9	78 604

The substance/substance group *Methylcellulose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.3913 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.6471 %)
Type C	100.0000 % (> 99.8817 %)	97.2308 % (> 96.3077 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21702	20919	9.51	50.12
20705	20705	0.00	33.72
21570	20705	9.35	34.20
22609	20705	10.16	32.29
20919	20919	0.00	49.01
22457	22457	0.00	33.80

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Methylcobalamin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20743-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Methylcobalamin

Special notes

When selecting the *Methylcobalamin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Methylcobalamin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Methylcobalamin	1207019-01	20743	40	1402501
Euro OTC	Methylcobalamin	1401032-01	21721	40	8778
Euro OTC	Methylcobalamin	1510002	22234	40	20151201*
Euro OTC	Methylcobalamin	1401032	22239	40	20151201*
Euro OTC	Methylcobalamin	1601043	22379	40	20160209*
Euro OTC	Methylcobalamin	1804006	24072	40	20180420*
Euro OTC	Methylcobalamin	1809001	24311	40	20180925*

Validation samples

A total of 280 317 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 *Methylcobalamin*. These samples are listed above in the [calibration samples](#) section.
- 74 216 spectra from a total of 1616 batches from further 372 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 5 reference samples from the substance/substance group *Methylcobalamin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Methylcobalamin	1401032-01	21721 [†]	20
Euro OTC	Methylcobalamin	1510002	22234 [†]	20
Euro OTC	Methylcobalamin	1401032	22239 [†]	20
Euro OTC	Methylcobalamin	1601043	22379 [†]	20
Euro OTC	Methylcobalamin	1711031	23885	40

- 126 772 spectra from a total of 2784 batches from further 781 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*.

- 3 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Methylcobalamin*.

Supplier	Substance	Batch	Spectra
Euro OTC	Methylcobalamin	1601043-02	1
Euro OTC	Methylcobalamin	1711031-01	1
Euro OTC	Methylcobalamin	1804006-01	1

- 78 926 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Methylcobalamin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methylcobalamin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 216
Type B	0	116	4	126 772
Type C	0	3	0	78 926

The substance/substance group *Methylcobalamin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	96.6667 % (> 94.1667 %)
Type C	100.0000 % (> 99.8821 %)	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
22234	22234	0.00	15.76
20743	20743	0.00	26.15
22239	22239	0.00	25.84
22379	22379	0.00	19.96
24072	24072	0.00	16.70
24311	24311	0.00	20.69
21721	21721	0.00	16.46

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Methylprednisolone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20953-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Methylprednisolone; Methylprednisolonum

Special notes

When selecting the *Methylprednisolone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Methylprednisolone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Methylprednisolone	13G19-N05	20953	40	1402438
Fagron	Methylprednisolone	15I04-B05-311572	22275	30	AR-16-FG-009102-01
Fagron	Methylprednisolone	15I04-B05-311572	22354	30	20151026
Fagron	Methylprednisolone	15I04-B05-311572	22275SI	30	AR-16-FG-009102-01
Fagron	Methylprednisolone	15I04-B05-311572	22354SI	30	20151026

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 5 reference samples from the substance/substance group *Methylprednisolone*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1621 batches from further 372 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 [†].

- 250 spectra of 9 reference samples from the substance/substance group *Methylprednisolone*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Methylprednisolone	12D17-N04	20650	40
Fagron	Methylprednisolone	15I04-B05-311572	22275 [†]	15
Fagron	Methylprednisolone	15I04-B05-311572	22354 [†]	15
Fagron	Methylprednisolone	15L15-B01-321887	23229	40
Fagron	Methylprednisolone	18A03-B05-345742	23997	40
Fagron	Methylprednisolone	15I04-B05-311572	22275SI [†]	15
Fagron	Methylprednisolone	15I04-B05-311572	22354SI [†]	15
Fagron	Methylprednisolone	15L15-B01-321887	23229SI	30
Fagron	Methylprednisolone	18A03-B05-345742	23997SI	40

- 126 642 spectra from a total of 2785 batches from further 781 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*.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Methylprednisolone*.

Supplier	Substance	Batch	Spectra
Fagron	Methylprednisolone	12D17-N04	1

- 78 928 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Methylprednisolone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methylprednisolone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	250	0	126 642
Type C	0	1	0	78 928

The substance/substance group *Methylprednisolone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.8830 %)	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
22275	22275	0.00	34.63
20953	20953	0.00	29.99
22354	22275	3.72	35.91

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Metoclopramide hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	21662-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metoclopramide hydrochloride; Metoclopramidi hydrochloridum

Special notes

When selecting the *Metoclopramide hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Metoclopramide hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metoclopramide h...	14193102	21662	40	AR-15-FG-002889-01
Caelo	Metoclopramide h...	14193102	21746	40	20140725
Caelo	Metoclopramide h...	15421101	23234	40	20160226

Validation samples

A total of 280 317 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 *Metoclopramide hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1621 batches from further 372 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 *Metoclopramide hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metoclopramide hydrochloride	14193102	21662 [†]	20
Caelo	Metoclopramide hydrochloride	14193102	21746 [†]	20
Caelo	Metoclopramide hydrochloride	15421102	23718	40
Gatt-Koller	Metoclopramide hydrochloride	20170236	24410	40

- 126 772 spectra from a total of 2786 batches from further 781 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.

- 17 spectra from 17 *Apo-Ident* customers from 3 batches from the substance/substance group *Metoclopramide hydrochloride*.

[†]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&lorenz,Phoenix	Metoclopramide hydrochloride	14193101	1
Caelo	Metoclopramide hydrochloride	14193101	1
Caelo	Metoclopramide hydrochloride	15227001	14
Caelo	Metoclopramide hydrochloride	3414U-018969	1

- 78 912 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Metoclopramide hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metoclopramide hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	120	0	126 772
Type C	0	17	0	78 912

The substance/substance group *Metoclopramide hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
21662	21662	0.00	49.84
21746	21662	4.97	50.21
23234	21662	6.68	49.23

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Metoprolol tartrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21753-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Metoprolol tartrate; Metoprololi tartras

Special notes

When selecting the *Metoprolol tartrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Metoprolol tartrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Inresa	Metoprolol tartr...	309905RII	21753	40	AR-15-FG-006635-01
Inresa	Metoprolol tartr...	405005RII	21805	40	20140430
Fagron	Metoprolol tartr...	16E31-B03-327107	22944	40	20160627

Validation samples

A total of 280 317 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 *Metoprolol tartrate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Metoprolol tartrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Inresa	Metoprolol tartrate	309905RII	21753 [†]	20
Inresa	Metoprolol tartrate	405005RII	21805 [†]	20
Inresa	Metoprolol tartrate	405005RIIC	22908	40
Fagron	Metoprolol tartrate	16E31-B03-327107	22927	40
Fagron	Metoprolol tartrate	16E31-B03-327107	22943	40

- 126 732 spectra from a total of 2785 batches from further 781 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 19 *Apo-Ident* customers from 18 batches from the substance/substance group *Metoprolol tartrate*.

[†]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
Inresa	Metoprolol tartrate	4050005RIIB	1
Th. Geyer	Metoprolol tartrate	56392-17-7	1
Antares	Metoprolol tartrate	1014Q-07308	1
Sigma-Aldrich GmbH	Metoprolol tartrate	LRAA6905	4
Inresa	Metoprolol tartrate	504005RIIC/29082016	1
Fagron	Metoprolol tartrate	16E31-B03-325535	1
Fagron	Metoprolol tartrate	16E31-B03-327107	23
Sigma Adrich/Alliance H.	Metoprolol tartrate	PHR1076	1
Audor Pharma	Metoprolol tartrate	APMTP00117MT	4
Sidonia	Metoprolol tartrate	405005RIIC/09062017	1
Fagron	Metoprolol tartrate	17G03-B09-340197	1
Andor	Metoprolol tartrate	APMTP0117MT	1
Audor Pharma	Metoprolol tartrate	APMTP0C117MT	1
Fagron	Metoprolol tartrate	17G03-B09-347089	1
Klosterring	Metoprolol tartrate	17G03-B09-345301	1
Caelo	Metoprolol tartrate	17G03-B09-351672	1
Fagron	Metoprolol tartrate	17G03-B09-350669	1
Audor Pharma	Metoprolol tartrate	MTP00117MT	1

- 78 883 spectra from 565 *Apo-Ident* customers from a total of 26 119 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Metoprolol tartrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metoprolol tartrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	0	126 732
Type C	0	43	3	78 883

The substance/substance group *Metoprolol tartrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	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
22944	21753	9.06	58.53
21753	21753	0.00	53.79
21805	21753	2.46	52.39

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Metronidazole**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20001-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Metronidazole; Metronidazolum

Special notes

When selecting the *Metronidazole* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metronidazole	12110410	20857	40	20120515
Fagron	Metronidazole	13D10-N02	21212	40	20130516
Euro OTC	Metronidazole	1212030-02	21213	40	20130627
Caelo	Metronidazole	13095007	21356	40	20130426
Euro OTC	Metronidazole	1508004	21881	40	20150819*
Caelo	Metronidazole	160892	22472	40	20160413*

Validation samples

A total of 280 317 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 *Metronidazole*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 [†].

- 500 spectra of 14 reference samples from the substance/substance group *Metronidazole*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metronidazole	13095005	21214	40
Caelo	Metronidazole	13095007	21360	40
Euro OTC	Metronidazole	1508004	21881 [†]	20
Caelo	Metronidazole	160892	22472 [†]	20
Euro OTC	Metronidazole	1609028	22751	40
Fagron	Metronidazole	16I19-B04-326155	22835	40
Euro OTC	Metronidazole	1612013	22917	40
Euro OTC	Metronidazole	1701039	23132	40
Euro OTC	Metronidazole	1707008	23542	30
Euro OTC	Metronidazole	1706022	23550	30
Caelo	Metronidazole	172905	23808	40
Euro OTC	Metronidazole	1802007	23946	40
Euro OTC	Metronidazole	1807039	24203	40
Euro OTC	Metronidazole	1901042	24449	40

- 126 392 spectra from a total of 2775 batches from further 781 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.

- 1769 spectra from 444 *Apo-Ident* customers from 447 batches from the substance/substance group *Metronidazole*.

Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	10368310	1
Anzag 21.10.14 EK 2.85	Metronidazole	13095007	1
Caelo	Metronidazole	11319810	2
Caelo	Metronidazole	10112907	1
Gehe	Metronidazole	10368318	1
Caelo	Metronidazole	11h11-n03	1
Spangropharm	Metronidazole	11319818	1
Caelo	Metronidazole	11319816	2
Euro OTC	Metronidazole	1109016-01	1
Caelo	Metronidazole	10368319	1
Caelo	Metronidazole	10368313	1
Caelo	Metronidazole	28061204	1
Caelo	Metronidazole	11319824	2
Fagron	Metronidazole	12F15-N04	7
Caelo	Metronidazole	607211870	1
Caelo	Metronidazole	11319819	1
Caelo	Metronidazole	11319807	1
Noweda	Metronidazole	11319818	1
Caelo	Metronidazole	12110405	8
Caelo	Metronidazole	11319818	2
Euro OTC	Metronidazole	1112028-01	4
Caelo	Metronidazole	12110414	3
Caelo	Metronidazole	11319825	2
Euro OTC	Metronidazole	1109030-01	5
Caelo	Metronidazole	11319823	5
Euro OTC	Metronidazole	1109030-02	1
Noweda	Metronidazole	12110404	1
Noweda	Metronidazole	12G04-N15	1
EuRho	Metronidazole	1109030-02	1
Caelo	Metronidazole	12110412	5
Caesar&lorenz,Phoenix	Metronidazole	12110410	1
Caelo	Metronidazole	1112028-01	1
Fagron	Metronidazole	12G04-N15	15
Caelo	Metronidazole	3112M-01870	1
Caelo	Metronidazole	12110413	4
Fagron	Metronidazole	11F15-N07	1
Anzag	Metronidazole	11373512	1
Caelo	Metronidazole	15121202	1
Euro OTC	Metronidazole	1112028-02	7
Fagron	Metronidazole	12a2o-n18	1
Caelo	Metronidazole	20140612-12	1
Caelo	Metronidazole	12110403	1
Fagron	Metronidazole	12D30-N03	4
EuRho	Metronidazole	110903002	1
Caelo	Metronidazole	102311870	1
Sanacorp	Metronidazole	12110422	1
Euro OTC	Metronidazole	20111025	1

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Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	12L17-N11	3
Caelo	Metronidazole	12110411	5
Caelo	Metronidazole	12110415	4
Caelo	Metronidazole	12110422	15
Euro OTC	Metronidazole	1109030-03	2
Fagron	Metronidazole	12L17N11	1
Caelo	Metronidazole	1109030-01	2
Fagron	Metronidazole	3212E01870	1
Caelo	Metronidazole	12110421	6
Fagron	Metronidazole	12L17-N11	14
Fagron	Metronidazole	12L17-N16	4
Fagron	Metronidazole	11J07-N07	1
Caelo	Metronidazole	12110105	1
Sanacorp	Metronidazole	12G04-N15	1
Euro OTC	Metronidazole	1212001-01	8
Fagron	Metronidazole	9041303	1
Fagron	Metronidazole	13B06-N03	10
Caelo	Metronidazole	12339501	7
Gehe	Metronidazole	12110422	1
vdl	Metronidazole	12110421	1
Gehe	Metronidazole	12110415	1
Fagron	Metronidazole	12L-N11	1
Caelo	Metronidazole	12339503	6
Caelo	Metronidazole	10368311	1
Caelo	Metronidazole	12110423	1
Caelo	Metronidazole	12339502	18
Noweda	Metronidazole	12339501	1
Euro OTC	Metronidazole	F120017	1
Phönix	Metronidazole	1109030-03	1
Caelo	Metronidazole	12339507	6
Gehe	Metronidazole	1112028-02	1
Caelo	Metronidazole	1239504	1
A.H. 19.02.13 ek: 5,86EUR	Metronidazole	12G04-N15	1
Caelo	Metronidazole	12339504	6
Euro OTC	Metronidazole	700837	1
Caelo	Metronidazole	2071304	1
Caelo	Metronidazole	2813E1870	1
Fagron	Metronidazole	12117-n11	1
Caelo	Metronidazole	12339510	9
Euro OTC	Metronidazole	121001-02	3
Phönix	Metronidazole	12L17-N11	1
Fargon	Metronidazole	13D08-N22	1
Fagron	Metronidazole	13D08N22	1
EuRho	Metronidazole	1212001-02	1
Fagron	Metronidazole	13D08-N22	6
Caelo	Metronidazole	121104085	1
Euro OTC	Metronidazole	1212030-01	3
Caelo	Metronidazole	12339508	4
Caelo	Metronidazole	121203001	2
Euro OTC	Metronidazole	1212001-02	12
Caelo	Metronidazole	2013U-01870	1
Fagron	Metronidazole	13B06N03	1
Caelo	Metronidazole	1201156	1
Caelo	Metronidazole	3947/V04/16	1
Caelo	Metronidazole	13095001	10
Fagron	Metronidazole	20121121	3
Caelo	Metronidazole	12339509	4
Caelo	Metronidazole	12339511	14
Euro OTC	Metronidazole	13B06-N03	1
Caelo	Metronidazole	10368318	1

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Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	12339519	12
Caelo	Metronidazole	12359501	1
Phoenix	Metronidazole		1
Alliance Healthcare	Metronidazole	12110415	1
Caesar&Loretz GmbH/Anzag	Metronidazole	12339511	1
Phönix	Metronidazole	121203001	1
Henry Lamotte	Metronidazole	1212001-02	1
Fagron	Metronidazole	10F23-N05	1
Caelo	Metronidazole	1210411	1
Sanacorp	Metronidazole	12339519	1
Fagron	Metronidazole	11C21-N01	1
Caelo	Metronidazole	12339520	4
Caelo	Metronidazole	14111304	1
Sanacorp	Metronidazole	39AKD15	1
Fagron	Metronidazole	20130906F	4
Fagron	Metronidazole	13J21-N07	34
Fagron	Metronidazole	12D30-N02	1
Phönix	Metronidazole	13J21-N07	1
Fagron	Metronidazole	112356	1
Caelo	Metronidazole	8012014B	1
Euro OTC	Metronidazole	1212030-02	7
Fagron	Metronidazole	PM41	1
Caelo	Metronidazole	12339526	1
Fagron	Metronidazole	13D10-N02	4
Fagron	Metronidazole	13J21N07	2
Caelo	Metronidazole	39/AKD16	1
Fagron	Metronidazole	12L17N16	1
Caelo	Metronidazole	18051201	1
Caelo	Metronidazole	13095003	10
Corden Pharma	Metronidazole	1212001-02	2
Euro OTC	Metronidazole	130704201	1
Caelo	Metronidazole	614U1870	1
Caelo	Metronidazole	13095005	4
Alliance Health 23.01.2...	Metronidazole	1212001-02	1
Caelo	Metronidazole	13095002	8
Caelo	Metronidazole	13095004	11
Fagron	Metronidazole	12d30-n03	1
Euro OTC	Metronidazole	1307002-01	11
Caelo	Metronidazole	7031401	1
Caelo	Metronidazole	1212030-21	1
Euro OTC	Metronidazole	1307042-01	8
Gehe am 04.02.14	Metronidazole	1212030-01	2
Phoenix	Metronidazole	121203002	1
Caelo	Metronidazole	13095006	6
Sanacorp	Metronidazole	13095002	1
Caelo	Metronidazole	12339521	1
Caelo	Metronidazole	1307042-01	1
Fagron	Metronidazole	13I10-N03	3
Caelo	Metronidazole	13095007	5
Caelo	Metronidazole	13095012	12
Alliance Health 20.05.2...	Metronidazole	1307042-01	2
Sanacorp	Metronidazole		1
Euro OTC	Metronidazole	1308704201	1
Euro OTC	Metronidazole	1307042-02	6
Cealo/Sanacorp	Metronidazole	13095003	1
Noweda	Metronidazole	13095012	1
GEHE 11.06.2014	Metronidazole	1307002-01	1
Caelo	Metronidazole	18071401	1
Caelo	Metronidazole	13095013	13
Caelo	Metronidazole	7071405	1

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Supplier	Substance	Batch	Spectra
Fagron	Metronidazole	13/21-N07	1
Caelo	Metronidazole	13095011	3
Fagron	Metronidazole	1414-B02-291237	1
Fagron	Metronidazole	13095002	1
Fagron	Metronidazole	14C14B02	3
Gehe	Metronidazole	1307002-01	1
Fagron	Metronidazole	13j21-n07	2
Caelo	Metronidazole	9715621	1
Caelo	Metronidazole	13095020	5
Caelo	Metronidazole	13214001	13
EuRho	Metronidazole	1406010-01	1
Caelo	Metronidazole	13J21-N07	1
Caelo	Metronidazole	12091403	1
Fagron	Metronidazole	14C14-B02-291276	2
Fagron	Metronidazole	14C14-B02-291237	8
Sanacorp	Metronidazole	39/AKD18	1
Fagron	Metronidazole	14B27-B31-291234	1
Fagron	Metronidazole	13j21-N07	1
Caelo	Metronidazole	27092014A	1
Fagron	Metronidazole	14C14-B02-291239	6
Caelo	Metronidazole	13214002	17
Euro OTC	Metronidazole	1406010-01	18
anzag	Metronidazole	14C14-B02-291276	2
Ichthyol Gesellschaft	Metronidazole	13095005	1
Caelo	Metronidazole	1307002	1
Fagron	Metronidazole	14c14b02291276	1
Fagron	Metronidazole	14C14-B02	4
Kuerzel	Metronidazole	1307002-02	1
Caelo	Metronidazole	13095019	7
Fagron	Metronidazole	14C14-B02-291275	4
Caelo	Metronidazole	132140022	1
Caelo	Metronidazole	13214003	11
Fagron	Metronidazole	12f15-n04	1
EuRho/Phönix	Metronidazole	1307002-01	1
Fagron	Metronidazole	20140131F	3
Fagron	Metronidazole	14c14-b02-291276	2
Fagron	Metronidazole	14C14-B02-291238	2
Caelo	Metronidazole	13095017	2
Gehe	Metronidazole	1307002-02	1
Euro OTC	Metronidazole	140601001	2
Fagron	Metronidazole	14c14-b02-291239	1
Euro OTC	Metronidazole	1407003-01	5
Euro OTC	Metronidazole		1
Caelo	Metronidazole	13214009	7
Fagron	Metronidazole	14C14-Bo2-291276	1
Caelo	Metronidazole	13095018	6
Caelo	Metronidazole	23011504	1
Fagron	Metronidazole	20140131f	1
Fagron	Metronidazole	14C14B02-291276	2
Caelo	Metronidazole	2022015B	1
Caelo	Metronidazole	1307002-02	1
Caelo	Metronidazole	13214010	4
Caelo	Metronidazole	14C14-B02-291276	1
Caesar & Lorenz	Metronidazole	13095013	1
Fagron	Metronidazole	14c14-b02-291275	1
Caelo	Metronidazole	13214014	9
Euro OTC	Metronidazole	1307002-02	1
Fagron	Metronidazole	14C14-B02-291241	1
Caelo	Metronidazole	13214011	1
Caelo	Metronidazole	13214012	3

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Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	13214016	2
Sanacorp 02.03.15	Metronidazole	13214009	1
Euro OTC	Metronidazole	1412016-01	12
Caelo	Metronidazole	13214017	3
Gehe01/2018	Metronidazole	14C14-B02-291237	1
Euro OTC	Metronidazole	1407003	1
Fagron	Metronidazole	172939-B01-295547	1
Fagron	Metronidazole	14C14-B291237	1
Gehe	Metronidazole	1407003-01	2
Caelo	Metronidazole	13041503	1
Euro OTC	Metronidazole	13070002-02	1
Caelo	Metronidazole	1412016-01	4
Hubei Hongyuan	Metronidazole	140700301	1
Phönix	Metronidazole	13214017	2
Fagron	Metronidazole	14C14-B02291238	1
Fagron	Metronidazole	14C14-B02-296437	10
Fagron	Metronidazole	14C14-802-291237	1
Caelo	Metronidazole	14C14-B02-291239	1
Caelo	Metronidazole	13214015	8
Eurho	Metronidazole	1406010-01	1
Anzag;14,21EUR;16.04.15	Metronidazole	13214012	1
Caelo	Metronidazole	1407003-01	1
Caelo	Metronidazole	113214021	1
Caelo	Metronidazole	13214013	1
Caelo	Metronidazole	1321409	1
Caelo	Metronidazole	11F15-N07	1
Euro OTC	Metronidazole	14120601	1
Fargon	Metronidazole	14c14-b02-291238	1
Caelo	Metronidazole	14C14-B02-291237	1
Fagron	Metronidazole	14C14-B02-300182	3
Phönix Gotha	Metronidazole	13214017	1
Caelo	Metronidazole	13214019	6
Fagron	Metronidazole	14C14-B02-295603	1
Fagron	Metronidazole	1220141155F	2
Fagron	Metronidazole	15A20-B07-303294	2
Fagron	Metronidazole	15A20-B07-303294Mg	1
Caelo	Metronidazole	39/AKD4	1
Caelo	Metronidazole	14B27-B31-291230	1
Euro OTC	Metronidazole	140700301	1
Caelo	Metronidazole	13214024	3
Fagron	Metronidazole	14C14-B02-2911239	1
Fagron	Metronidazole	15A20-B07-303295	1
Euro OTC	Metronidazole	15a20-b07-303294	1
Caelo	Metronidazole	14b27-b31-291230	1
Caelo	Metronidazole	14c14-b01-295545	1
Fagron	Metronidazole	14-C14-B02-296437	1
Caelo	Metronidazole	13214018	4
Fagron	Metronidazole	14B27-B31-291235	1
Fagron	Metronidazole	140700301	1
Caelo	Metronidazole	13214025	6
Caelo	Metronidazole	13214021	1
Noweda	Metronidazole	1407003-01	2
Caelo	Metronidazole	13214029	8
Euro OTC	Metronidazole	140700302	2
Fagron	Metronidazole	1412016-01	1
Euro OTC	Metronidazole	1407003-02	7
Caelo	Metronidazole	12081507	1
Caelo	Metronidazole	15215104	5
Fagron	Metronidazole	15A20-B07-308196	3
Sanacorp	Metronidazole	39/AKD6	1

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Supplier	Substance	Batch	Spectra
Noweda	Metronidazole	13214025	1
Fagron	Metronidazole	14C14-B01-306363	4
Caelo	Metronidazole	15215107	1
Gatt-Koller	Metronidazole	497/03151015	1
Caelo	Metronidazole	15215108	8
Fagron	Metronidazole	15A20-B07-308525	6
Euro OTC	Metronidazole	1412016-02	20
Caelo	Metronidazole	15A20-B07-303297	1
Caelo	Metronidazole	15215103	4
Fagron	Metronidazole	13/21-N7	2
Fagron	Metronidazole	15A20-B07-308791	3
Caelo	Metronidazole	15215106	5
Fagron	Metronidazole	15A20-B07	1
Gatt-Koller	Metronidazole	606293914	1
Euro OTC	Metronidazole	1505024-01	10
Fagron	Metronidazole	15A20-B07-303293	8
Gatt-Koller	Metronidazole	497/03151515	1
Sanacorp 27.10.15	Metronidazole	15A20-B07-303298	1
Caelo	Metronidazole	15253001	10
Fagron	Metronidazole	14C14-B01	1
Fagron	Metronidazole	15a20-b07-308196	1
Bombastus	Metronidazole	123Validierung	1
Fischer/Gehe	Metronidazole	15A20-B07-308525	1
Fagron	Metronidazole	15a20-b07-308791	1
ACM	Metronidazole		1
Caelo	Metronidazole	15253003	7
Bombastus	Metronidazole	13214018	1
Fagron	Metronidazole	14c14-B01-295545	1
Caelo	Metronidazole	15253013	9
Gatt-Koller	Metronidazole	497/03154015	1
Fagron	Metronidazole	15A20Bo7308196	1
Euro OTC	Metronidazole	1508004-01	23
Caelo	Metronidazole	15215105	1
Eurimpharm	Metronidazole	140601001	1
Caelo	Metronidazole	15253002	2
Caelo	Metronidazole	1412016-02	1
Caesar&Loretz GmbH/Sana...	Metronidazole	15253003	1
Caelo	Metronidazole	15253004	13
Caelo	Metronidazole	1523013	1
Caelo	Metronidazole	15253005	2
Fagron	Metronidazole	15A20-B07-303298	8
Fagron	Metronidazole	141C14-B02-296437	1
Caelo	Metronidazole	15253006	7
Gehe	Metronidazole	1505024-01	1
Fagron	Metronidazole	14C14-B01-309058	2
Fagron	Metronidazole	15A20B07308525	1
Fagron	Metronidazole	15A20/B07-303298	1
Caelo	Metronidazole	15253011	8
Fagron	Metronidazole	12A20-B07-303298	1
Fagron	Metronidazole	14C14-B01-295548	1
Fagron	Metronidazole	15A20-B07-312057	3
Caelo	Metronidazole	1523006	1
Caelo	Metronidazole	15253015	8
Fagron	Metronidazole	15A20-B07312057	1
Caelo	Metronidazole	15253013/2016030911	1
Caelo	Metronidazole	15253007	11
Fagron	Metronidazole	15A20-B07-312225	3
Caelo	Metronidazole	15253016	10
Euro OTC	Metronidazole	10800401	1
Fagron	Metronidazole	15a20b07303298	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Metronidazole	1412016	1
Caelo	Metronidazole	15253017	11
Fagron	Metronidazole	15A20-B07-31225	1
Fagron	Metronidazole		1
Euro OTC	Metronidazole	1508004-02	10
	Metronidazole	15253007	2
Caelo	Metronidazole	15253018	5
EuRho	Metronidazole	1407003-01	1
Caesar & Loretz GmbH	Metronidazole	15253017	1
Phönix	Metronidazole	15253018	1
Euro OTC	Metronidazole	150804-01	1
Caelo	Metronidazole	1523017	1
Euro OTC	Metronidazole	1505024-02	6
Caelo	Metronidazole	15253020	5
Euro OTC	Metronidazole	1508004	1
Caelo	Metronidazole	15253019	3
Caelo	Metronidazole	15A20-B07-303298	1
Caelo	Metronidazole	1508004-01	1
Caelo	Metronidazole	15253021	4
Caelo	Metronidazole	15258016	1
Caelo	Metronidazole	15253022	3
Caelo	Metronidazole	15253024	10
Caelo	Metronidazole	1523026	1
Euro/ Sanacorp	Metronidazole	150800402	1
Caelo	Metronidazole	15253026	17
Euro OTC	Metronidazole	1505024-03	2
Caelo	Metronidazole	1505024-02	2
Euro OTC	Metronidazole	150800401	1
Caelo	Metronidazole	15253029	2
Euro OTC	Metronidazole	150502401	1
phönix	Metronidazole	15253026	1
Caelo	Metronidazole	15253027	10
Euro OTC	Metronidazole	150800	1
Noweda	Metronidazole	1505024-03	1
Euro OTC	Metronidazole	300915ME	1
Phoenix	Metronidazole	16089201	1
Fagro	Metronidazole	14C14-B01-295548	1
Caelo	Metronidazole	15253028	9
Caelo	Metronidazole	16089201	4
Caelo	Metronidazole		3
Caelo	Metronidazole	16089202	9
Bombastus	Metronidazole	15253032	1
Caelo	Metronidazole	16089209	6
Farchemia S.R.L./ Caesa...	Metronidazole	15253032	1
ALH	Metronidazole	1609028-01	1
Euro OTC	Metronidazole	1609028-01	19
Caelo	Metronidazole	15253032	9
Fagron	Metronidazole	16D15-B50-324137	1
Caelo	Metronidazole	15253033	4
Fagron	Metronidazole	16I19-B04-326150	2
Fagron	Metronidazole	16/19-B04-326150	6
Caelo	Metronidazole	16089212	14
Caelo	Metronidazole	16/19-B04-326155	1
Caelo	Metronidazole	160902801	1
Fagron	Metronidazole	16I19-B04-326155	3
Euro OTC	Metronidazole	1503004-01	1
Gehe	Metronidazole	16H15-B50-326734	1
Fagron	Metronidazole	19119-B04-326154	1
Caelo	Metronidazole	16089213	14
Phoenix 12.10.2016 6,63EUR	Metronidazole	15253027	1

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Supplier	Substance	Batch	Spectra
EURO / Sanacorp	Metronidazole	160902801	1
Caelo	Metronidazole	1508004-02	1
Euro/Sanacorp	Metronidazole	1609028	1
Farchemia S. r. l.	Metronidazole	1609028-01	1
Caelo	Metronidazole	16089216	5
Caelo	Metronidazole	16089218	7
Caelo	Metronidazole	16089217	6
Fagron	Metronidazole	16/19-B04-326155	2
Euro OTC	Metronidazole	150502402	1
Fagron	Metronidazole	16I19-B04	3
Fagron	Metronidazole	16I19-B04-326150	1
Phönix	Metronidazole	16089212	1
Caelo	Metronidazole	16089215	11
Fagron	Metronidazole	16I19-B04-326151	4
Fagron	Metronidazole	16/19bo4326155	1
AHD 03.02.17	Metronidazole	16089212	1
Caelo	Metronidazole	1609028-01	4
Bombastus	Metronidazole	1609028-01	1
Ichthyol/ALH	Metronidazole	1609028-02	1
Euro/Noweda	Metronidazole	1609028-01	1
GEHE	Metronidazole	15253032	1
Noweda/Wepa	Metronidazole	13214017	1
Caelo	Metronidazole	23021713	1
Caelo	Metronidazole	16089219	5
Fagron	Metronidazole	16I19-B04-326152	2
Caelo	Metronidazole	16089215/1140217	1
Euro OTC	Metronidazole	1609028	2
Caelo	Metronidazole	16089225	1
Euro OTC	Metronidazole	1606028	1
Fagron	Metronidazole	16I19-B04-329167	2
Fagron	Metronidazole	160902	1
Caelo	Metronidazole	1619-b04-326150	1
Fagron	Metronidazole	1609028-01	2
Anzag	Metronidazole	15253022	1
Euro OTC	Metronidazole	1612013-01	12
Fagron	Metronidazole	16/19-B04-326154	1
Fagron	Metronidazole	16/19-B04	1
Caelo	Metronidazole	16089221	3
Fagron	Metronidazole	16J19-B04-326151	1
Euro OTC	Metronidazole	1609028-02	7
Caelo	Metronidazole	16089224	3
Caelo	Metronidazole	16/19-B04-326150	1
Euro OTC	Metronidazole	13214010	1
Caelo	Metronidazole	16089220	12
Caelo	Metronidazole	16089223	3
Ebert-Jacobi	Metronidazole	16089224	1
Fagron	Metronidazole	16/16-B04-326151	1
Euro OTC	Metronidazole	C04-160812	1
Euro OTC	Metronidazole	1701039-01	25
Caelo	Metronidazole	16089123	1
Caelo	Metronidazole	16089222	6
Noweda	Metronidazole	160902802	1
Caelo	Metronidazole	16051703	1
Fagron	Metronidazole	16/19-B04-329167	1
Euro OTC	Metronidazole	161201301	1
Fagron	Metronidazole	1619b04326155	1
GEHE	Metronidazole	16089216	1
EuRho	Metronidazole	1701039-01	1
Farchemia/Phönix	Metronidazole	1609028-02	1
Fagron	Metronidazole	16/19-B04-326152	1

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Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	16089228	5
Caelo	Metronidazole	16089229	4
Fagron	Metronidazole	16/19-B04-329168	3
Fagron	Metronidazole	17/19-304-329168	1
Apotheke an der Bornhei...	Metronidazole	16089223	1
Caeolo/Phönix	Metronidazole	16089228	1
Fagron	Metronidazole	606/10072017	1
Caelo	Metronidazole	16056235	1
Caelo	Metronidazole	160892365302	1
Fagron	Metronidazole	16I19-B04-329159	1
Caelo	Metronidazole	16089235	2
Sanacorp	Metronidazole	16I19-B04-329159	1
Caelo	Metronidazole	17058001	4
Klosterring	Metronidazole	16089235	1
Caelo	Metronidazole	16089228-20170818Ma4	1
Caelo	Metronidazole	17058002	5
Caelo	Metronidazole	16089236	2
Delta	Metronidazole	17058001	1
Noweda	Metronidazole	17058005	2
Fagron	Metronidazole	16/19-b04-329168	1
Caelo	Metronidazole	7091714	1
Caelo	Metronidazole	170580001	1
Sanacorp	Metronidazole	17058002	1
Caelo	Metronidazole	1612013-01	1
Fagron	Metronidazole	1619-B04-326150	1
Caelo	Metronidazole	17058005	6
Fagron	Metronidazole	16I19-B04-329165	1
Caelo	Metronidazole	17058004	2
GEHE	Metronidazole	16089229	1
Caelo	Metronidazole	17058003	5
Euro OTC	Metronidazole	1703028-01	1
Gatt-Koller	Metronidazole	3728/11162017	1
Euro OTC	Metronidazole	17058005	1
Caelo	Metronidazole	17058019	7
Apoident,Phönix, 09.11....	Metronidazole	1701039-01	1
Caelo	Metronidazole	161201301	1
Caelo	Metronidazole	17058012	10
Kehr	Metronidazole	17058003	1
Frago/Noweda	Metronidazole	16I19-B04-329163	1
Caelo	Metronidazole	17058013	8
Caelo	Metronidazole	170580035444	1
Noweda	Metronidazole	1619-B04-329166	1
Noweda	Metronidazole	17058013	1
Caelo	Metronidazole	17058012/2231117	1
Caelo	Metronidazole	16089231	2
Phönix	Metronidazole	17058016	1
Gehe	Metronidazole	17058016	1
Caelo	Metronidazole	17058016	10
Caelo	Metronidazole	17058010	4
GEHE	Metronidazole	17058013	1
Caelo	Metronidazole	1701039-01	1
Fagron	Metronidazole	17058013	1
Sanacorp	Metronidazole	16I19-B04-329160	1
Fagron	Metronidazole	16I19-B04-329160	2
Fagron	Metronidazole	15A20-B07-308198	1
Phönix	Metronidazole	17058003	1
Euro OTC	Metronidazole	1707008-01	15
Caelo	Metronidazole	17058015	4
Caelo	Metronidazole	1705801	1
Euro OTC	Metronidazole	169028-01	1

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Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	170580123	1
Caelo	Metronidazole	17058027	2
Caelo	Metronidazole	17058017	9
Phoenix	Metronidazole	17058027	1
Phoenix/Cealo	Metronidazole	17058016/0818E-0187	1
Caelo	Metronidazole	17058011	3
Caelo	Metronidazole	17058018	9
Noweda	Metronidazole	1701039-01	1
Fagron	Metronidazole	16/19-B04-326151	1
Fiebig	Metronidazole	17058027	1
Caelo	Metronidazole	17058014	8
Euro OTC	Metronidazole	1701039	1
Caelo	Metronidazole	17058026	7
Caelo	Metronidazole	170580165554	1
Caelo	Metronidazole	17058013-20180404Ma4	1
Fagron	Metronidazole	16I19-B04-329162	1
Sanacorp	Metronidazole	1707008-01	1
GEHE	Metronidazole	17058015	1
Caelo	Metronidazole	280218010	1
Noweda	Metronidazole	17058014	1
Fagron	Metronidazole	16/19-B04-329160	1
Sanacorp	Metronidazole	1701039-01	1
Fagron	Metronidazole	605021726	2
Bombastus	Metronidazole	18026401	1
Caelo	Metronidazole	17290506	9
Caelo	Metronidazole	16/19-B04-329160	1
Sanacorp	Metronidazole	17058018	1
Sanacorp	Metronidazole	17C10-B04-338707	1
17270001	Metronidazole	17058026	1
EuRho/Noweda	Metronidazole	180601M1706022-01	1
Caelo	Metronidazole	1061804	2
Caelo	Metronidazole	18026401	5
Fagron	Metronidazole	17C10	1
Caelo	Metronidazole	18061803	1
Caelo	Metronidazole	17058013-20180619Ma6	1
Caelo	Metronidazole	1707008-01	1
Caelo	Metronidazole	17290515	3
Delta	Metronidazole	17290503	2
Caelo	Metronidazole	17290503	7
Sanacorp	Metronidazole	17C10-B04-346280	2
Fagron	Metronidazole	17C10-B04-346275	1
Caelo	Metronidazole	17290509	1
Cealo/Gehe	Metronidazole	17290506	1
EuRho	Metronidazole	1707008-01	1
Caelo	Metronidazole	17290512	6
Sanacorp	Metronidazole	17290512	1
Caelo	Metronidazole	17290507	4
Fagron	Metronidazole	17C10-B04-346276	1
Caelo	Metronidazole	172905125723	1
Caelo	Metronidazole	1790512	1
Euro OTC	Metronidazole	1807039-01	5
Fagron	Metronidazole	17C10-B04-346277	2
Euro OTC	Metronidazole	170700801	1
Euro OTC	Metronidazole	1707008-02	1
Caelo	Metronidazole	17290513	1
Caelo	Metronidazole	17290504	6
Euro OTC	Metronidazole	1706022-01	2
Gehe 23.11.18	Metronidazole	1706022-02	1
Caelo	Metronidazole	17290517	5
Sanacorp	Metronidazole	601021826	1

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Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	17290518	8
Sanacorp	Metronidazole	17290518	1
Caelo	Metronidazole	19011909	1
Kehr	Metronidazole	17290512	1
Caelo	Metronidazole	17290527	1

- 77 160 spectra from 565 *Apo-Ident* customers from a total of 25 699 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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* can clearly be 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* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	500	0	126 392
Type C	0	1678	91	77 160

The substance/substance group *Metronidazole* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.8000 %)
Type C	100.0000 % (> 99.8817 %)	94.8559 % (> 94.6863 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
20857	22472	11.04	77.92
21212	21881	4.80	76.82
21213	21881	3.09	76.60
21356	21881	4.94	77.14
21881	21881	0.00	76.81
22472	22472	0.00	77.20

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Miconazole nitrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20210-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Miconazole nitrate; Miconazoli nitras

Special notes

When selecting the *Miconazole nitrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Miconazole nitrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Miconazole nitrate	13D22-N14	20817	95	20130529
Caelo	Miconazole nitrate	13185601	20875	40	20130704
Caelo	Miconazole nitrate	13352802	21350	39	1412250
Euro OTC	Miconazole nitrate	1307025-02	21649	40	20130806
Euro OTC	Miconazole nitrate	1509014	21900	40	20150930*
Caelo	Miconazole nitrate	161447	22630	40	20160617*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 294 spectra of 6 reference samples from the substance/substance group *Miconazole nitrate*. These samples are listed above in the [calibration samples](#) section.
- 74202 spectra from a total of 1617 batches from further 372 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 [†].

- 808 spectra of 21 reference samples from the substance/substance group *Miconazole nitrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Miconazole nitrate	13D22-N14	20817 [†]	5
Caelo	Miconazole nitrate	13185601	20905	80
Caelo	Miconazole nitrate	13352802	21351	40
Euro OTC	Miconazole nitrate	1307025-02	21649 [†]	20
Euro OTC	Miconazole nitrate	1509014	21900 [†]	20
Euro OTC	Miconazole nitrate	1604004	22522	40
Euro OTC	Miconazole nitrate	1607004	22671	40
Euro OTC	Miconazole nitrate	1611024	22920	40
Euro OTC	Miconazole nitrate	1705039	23429	40
Caelo	Miconazole nitrate	172175	23662	30
Euro OTC	Miconazole nitrate	1710020	23775	40
Euro OTC	Miconazole nitrate	1803028	24071	40
Euro OTC	Miconazole nitrate	1811015	24338	40
Caelo	Miconazole nitrate	182821	24388	40
Caelo	Miconazole nitrate	13185601	20875SI	60
Euro OTC	Miconazole nitrate	1307025-02	21649SI	37
Euro OTC	Miconazole nitrate	1509014	21900SI	53
Euro OTC	Miconazole nitrate	1604004	22522SI	36
Caelo	Miconazole nitrate	161447	22630SI	40
Euro OTC	Miconazole nitrate	1607004	22671SI	30
Euro OTC	Miconazole nitrate	1611024	22920SI	37

*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*).

- 126 084 spectra from a total of 2774 batches from further 781 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.

- 980 spectra from 275 *Apo-Ident* customers from 244 batches from the substance/substance group *Miconazole nitrate*.

Supplier	Substance	Batch	Spectra
Caelo	Miconazole nitrate	11104113	1
Caelo	Miconazole nitrate	11104109	2
Caelo	Miconazole nitrate	11324902	1
Fagron	Miconazole nitrate	27061202	1
Caesar & Loretz GmbH, 4...	Miconazole nitrate	11324904	1
Caelo	Miconazole nitrate	11324901	1
Caelo	Miconazole nitrate	11104114	1
Caelo	Miconazole nitrate	11104103	2
Caelo	Miconazole nitrate	11324905	4
Fagron	Miconazole nitrate	20081201	1
Fagron	Miconazole nitrate	12A16-N02	2
Caelo	Miconazole nitrate	11324912	2
Fagron	Miconazole nitrate	12H10-N02	4
Fagron	Miconazole nitrate	12/21-M03	1
Caelo	Miconazole nitrate	11324909	1
Caelo	Miconazole nitrate	12243803	9
Caelo	Miconazole nitrate	12243801	3
Fagron	Miconazole nitrate	12K02-N06	7
Caelo	Miconazole nitrate	11243803	1
Caelo	Miconazole nitrate	12243802	4
Sanacorp	Miconazole nitrate	12243801	1
Caelo	Miconazole nitrate	9177904	1
Fagron	Miconazole nitrate	17011307	1
Caelo	Miconazole nitrate	12k02n06	1
Sanacorp	Miconazole nitrate	12243803	2
Caelo	Miconazole nitrate	11324913	1
Anzag	Miconazole nitrate	12243802	1
Caesar&Loretz GmbH D-4...	Miconazole nitrate	12243808	1
Caelo	Miconazole nitrate	12243805	6
Caelo	Miconazole nitrate	11104108	1
Bionorica /Phönix	Miconazole nitrate	12C13B03-279593	1
Anzag	Miconazole nitrate	12374301	3
Caelo	Miconazole nitrate	12243806	1
Fagron	Miconazole nitrate	2900/08/12	2
Caesar&lorenz,Phoenix	Miconazole nitrate	12374301	1
Caelo	Miconazole nitrate	12243808	9
Caelo	Miconazole nitrate	12374301	4
Caelo	Miconazole nitrate	12374307	14
Caelo	Miconazole nitrate		3
Caelo	Miconazole nitrate	1/AD1	1

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Hence, these spectra are not independent and are not of *Type B*.

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Supplier	Substance	Batch	Spectra
EUro/AHD	Miconazole nitrate	12243808	1
Caelo	Miconazole nitrate	28051306	1
Caelo	Miconazole nitrate	12374308	6
Caelo	Miconazole nitrate	4061304	1
Caesar und Loretz	Miconazole nitrate	12243805	1
Fagron	Miconazole nitrate	13E13-N08	2
Fagron	Miconazole nitrate	13A14B09283005	1
Fagron	Miconazole nitrate	13D22-N14	5
AHD	Miconazole nitrate	12374307	1
Caelo	Miconazole nitrate	13D22-N14	1
Fagron	Miconazole nitrate	13E13-N04	2
Caelo	Miconazole nitrate	13185603	10
Caelo	Miconazole nitrate	13185601	4
Alliance Healthcare	Miconazole nitrate	12374307	1
Caelo	Miconazole nitrate	13185602	6
Herstellung	Miconazole nitrate	13185602	1
Caelo	Miconazole nitrate	13185611	15
Fagron	Miconazole nitrate	13H28-N06	2
Caelo	Miconazole nitrate	AKD9	1
Fagron	Miconazole nitrate	13H28-N06	11
Fagron	Miconazole nitrate	4111301	1
Caelo	Miconazole nitrate	13185609	9
Fagron	Miconazole nitrate	31101306	1
Caelo	Miconazole nitrate	13H28-N06	1
Fagron	Miconazole nitrate	13A14-B09-287453	1
20; 04.12.13	Miconazole nitrate	13185611	2
Fagron	Miconazole nitrate	1328-N06	1
Phönix	Miconazole nitrate	13H28-N06	1
Caelo	Miconazole nitrate	13185610	6
Fagron	Miconazole nitrate	13A14-B09	2
Caesar&Loretz GmbH/Anzag	Miconazole nitrate	13185603	1
Caelo	Miconazole nitrate	13352801	17
Caelo	Miconazole nitrate	411092-2-P	1
Alliance Health 05.02.2...	Miconazole nitrate	13352801	2
Euro OTC	Miconazole nitrate	1307025-01	2
Sanacorp	Miconazole nitrate	13352801	1
Fagron	Miconazole nitrate	13A14-B09-287486	5
Fagron	Miconazole nitrate	13A14-B09-287487	3
Phoenix	Miconazole nitrate	13185611	1
Fagron	Miconazole nitrate	13H28N06	1
Caelo	Miconazole nitrate	13342801	1
Caelo	Miconazole nitrate	13352805	1
Caelo	Miconazole nitrate	13352802	16
Gehe am 29.04.2014	Miconazole nitrate	13352802	4
Fagron	Miconazole nitrate	14B18-B02-291248	6
Caelo	Miconazole nitrate	13185612	5
Sanacorp	Miconazole nitrate		1
Fagron	Miconazole nitrate	13A14-B09-287488	1
Phoenix	Miconazole nitrate	13352801	1
Fagron	Miconazole nitrate	14B18-B02-291249	1
Fagron	Miconazole nitrate	14B18-B02-291232	4
Caelo	Miconazole nitrate	13352806	11
Fagron	Miconazole nitrate	14B18-B02	4
Caesar&Loretz GmbH/Anzag	Miconazole nitrate	13352802	1
Fagron	Miconazole nitrate	14B18B02	1
Caelo	Miconazole nitrate	14B18-B02-291233	1
Fagron	Miconazole nitrate	14B18-B02-291250	1
Euro OTC	Miconazole nitrate	1307025-02	2
Caelo	Miconazole nitrate	14149305	1
Bombastus	Miconazole nitrate	13352806	1

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Supplier	Substance	Batch	Spectra
Caelo	Miconazole nitrate	14149302	15
Caelo	Miconazole nitrate	1419301	1
Caelo	Miconazole nitrate	14149301	14
Fagron	Miconazole nitrate	14D25-B06	4
Phoenix 21.10.14	Miconazole nitrate	14149301	1
Gehe	Miconazole nitrate	14149301	1
Caelo	Miconazole nitrate	1307025-02	1
Fagron	Miconazole nitrate	14D25-B06-294959	5
Caesar & Loretz GmbH Hi...	Miconazole nitrate	14149301	1
Fagron	Miconazole nitrate	2900/15/13	1
Caelo	Miconazole nitrate	1122014A	1
Caelo	Miconazole nitrate	13352811	5
Fagron	Miconazole nitrate	14B18-B02-291247	1
Fagron	Miconazole nitrate	2900/04/14	2
Caelo	Miconazole nitrate	14149303	5
Fagron	Miconazole nitrate	14149313	1
Fagron	Miconazole nitrate	14b18-b02-291247	1
Fagron	Miconazole nitrate	14D25-B06-294958	11
Caelo	Miconazole nitrate	14149310	6
Caelo	Miconazole nitrate	14D25-B06-294960	3
Caelo	Miconazole nitrate	14149308	11
Gehe	Miconazole nitrate	13352811	1
Caelo	Miconazole nitrate	1419310	1
Gehe 6.03.15	Miconazole nitrate	14149308	2
Fargon	Miconazole nitrate	14D25-B06-294959	1
Caelo	Miconazole nitrate	14149311	14
Fagron	Miconazole nitrate	14H06-B01-299813	3
Euro OTC	Miconazole nitrate	140902302	1
EuroPTC/Phönix	Miconazole nitrate	14149316	1
Euro OTC	Miconazole nitrate	1409023-02	4
GEHE 13.05	Miconazole nitrate	14149311	1
Noweda	Miconazole nitrate	14149311	1
Caelo	Miconazole nitrate	14149309	7
Caelo	Miconazole nitrate	14149318	19
Caelo	Miconazole nitrate	2900/10/14	1
Caelo	Miconazole nitrate	15A13-B07	1
Euro OTC	Miconazole nitrate	1409023-01	1
Fagron	Miconazole nitrate	14D25-B06-299790	2
Fagron	Miconazole nitrate	15A13-B07	7
Fagron	Miconazole nitrate	2900/16/14	2
Caelo	Miconazole nitrate	14149317	8
Fagron	Miconazole nitrate	14H06-B01-299799	7
Noweda	Miconazole nitrate	14149310	1
Caelo	Miconazole nitrate	14D25-B06-294959	1
Fagron	Miconazole nitrate	15A13-B07-306791	8
Fagron	Miconazole nitrate	15A13-B07-306791nron	1
Caesar&Loretz GmbH /Anzag	Miconazole nitrate	14149310	1
Caelo	Miconazole nitrate	29001614	1
Anzag	Miconazole nitrate	15A13-B07-308432	1
Euro OTC	Miconazole nitrate	1504903-01	1
Caelo	Miconazole nitrate	14H06-B01-299799	1
Fagron	Miconazole nitrate	14b18-B02-291231	1
Fagron	Miconazole nitrate	15I08-B07	3
Caelo	Miconazole nitrate	15137902	16
Caelo	Miconazole nitrate	15137906	1
Fagron	Miconazole nitrate	15A13-B07-307140	7
Anzag	Miconazole nitrate	15137902	1
Euro OTC	Miconazole nitrate	1504003-01	2
Fagron	Miconazole nitrate	15I08-B07-312321	7
Fagron	Miconazole nitrate	14d25-b06-299790	1

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Supplier	Substance	Batch	Spectra
Caelo	Miconazole nitrate	15137903	17
Caelo	Miconazole nitrate	15137911	1
Fagron	Miconazole nitrate	14H06-B01-299798	1
Fagron	Miconazole nitrate	2900/10/14	1
Caelo	Miconazole nitrate	15I08-B07-312317	3
Fagron	Miconazole nitrate	15a13-b07-307140	1
Caelo	Miconazole nitrate	151379	1
Fagron	Miconazole nitrate	15A13-807	1
Euro OTC	Miconazole nitrate	1509014-01	6
Fagron	Miconazole nitrate	15/08-B07-312317	1
Fagron	Miconazole nitrate	15108-B07-312321	1
Fagron	Miconazole nitrate	14H16-B01-299798	1
Fagron	Miconazole nitrate	15A13-B07-308432	2
Caelo	Miconazole nitrate	15137905	10
Fagron	Miconazole nitrate	1316Q-03451	1
Noweda	Miconazole nitrate	15137903	1
Caelo	Miconazole nitrate	2900/11/15	3
Fagron	Miconazole nitrate	15a13-b07-308432	1
Fagron	Miconazole nitrate	15I08-B07-315492	1
Ichthyol/Phoenix	Miconazole nitrate	16/098/M	1
Caelo	Miconazole nitrate	15137907	7
Fagron	Miconazole nitrate	15108-b07-312321	1
Euro OTC	Miconazole nitrate	1604004-01	4
Fagron	Miconazole nitrate	15I08-B07-3121321	1
Caelo	Miconazole nitrate	15137908	6
Fagron	Miconazole nitrate	15i08-b07-312317	1
Fagron	Miconazole nitrate	15137905	1
Fagron	Miconazole nitrate	15108-B07-318485	1
Caelo	Miconazole nitrate	15137909	6
Caelo	Miconazole nitrate	15I08-B07-315481	1
Bombastus	Miconazole nitrate	15I08-B07-318687	1
Caelo	Miconazole nitrate	15/05-B07-312317	1
Caelo	Miconazole nitrate	15137910	6
Fagron	Miconazole nitrate	15108-B07-315492	3
phönix	Miconazole nitrate	15137907	1
Fagron	Miconazole nitrate	15I08-B07-315481	1
Alliance H.	Miconazole nitrate	5137910	1
Caelo	Miconazole nitrate	15137913	3
Fagron	Miconazole nitrate		1
Caelo	Miconazole nitrate	15137914	4
Fagron	Miconazole nitrate	15I08-B07-318485	1
Caelo	Miconazole nitrate	15137915	3
Caelo	Miconazole nitrate	15I08-B07-318687	2
Caelo	Miconazole nitrate	15108-B07-314838	1
Caelo	Miconazole nitrate	15108-B07-318686	1
Fagron	Miconazole nitrate	15/08-B07-315481	1
Phoenix	Miconazole nitrate	15137915	1
Caelo	Miconazole nitrate	16144701	19
Euro OTC	Miconazole nitrate	1607004-01	6
Fagron	Miconazole nitrate	15i08-b07-315481	1
Caelo	Miconazole nitrate	16E04-B03-321367	1
Caelo	Miconazole nitrate	15/08-B07-315481	1
Caelo	Miconazole nitrate	16144703	10
Fagron	Miconazole nitrate	15/08-B07-318686	1
E+J, 27.09.2016	Miconazole nitrate	15137915	1
Fagron	Miconazole nitrate	15/08-b07-314838	2
phönix	Miconazole nitrate	16144701	2
Fagron	Miconazole nitrate	160711M	1
Fagron	Miconazole nitrate	15/08-b07-318687	1
Euro OTC	Miconazole nitrate	16144701	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz/AHC	Miconazole nitrate	15137910	1
Caelo	Miconazole nitrate	16e04-b03-321367	1
Fagron	Miconazole nitrate	15I08-B07-318686	2
Fagron	Miconazole nitrate	16E04-B03-322124	9
Caelo	Miconazole nitrate	16144702	18
Fagron	Miconazole nitrate	16E04-B03-322132	4
Fagron	Miconazole nitrate	16E04-B03	3
Fagron	Miconazole nitrate	1508-B07-318686	1
Fagron	Miconazole nitrate	16E04-B03-321354	1
Caelo	Miconazole nitrate	16E04-B03-322124	1
Fagron	Miconazole nitrate	15I08-B07-31485	1
Fagron	Miconazole nitrate	15/08-b07-315492	2
Caelo	Miconazole nitrate	16144704	10
Fagron	Miconazole nitrate	16144703	1
Caesar & Loretz GmbH	Miconazole nitrate	16144702	1
Euro OTC	Miconazole nitrate	16E04-B03-322124	1
Bombastus	Miconazole nitrate	15I08-B07-318686	1
Phönix	Miconazole nitrate	16E04-B03-322124	1
Fagron	Miconazole nitrate	16E04-B03-327362	6
Fagron	Miconazole nitrate	16E04-B03-322131	3
Fagron	Miconazole nitrate	2900/03/16	1
Fagron	Miconazole nitrate	15/08-B07-316911	1
Caelo	Miconazole nitrate	16144710	13
Phönix	Miconazole nitrate	16E04-B03-322131	1
Euro OTC	Miconazole nitrate	1611024-01	5
Fagron	Miconazole nitrate	15I08-B07-215492	1
Gehe/Ichthylol	Miconazole nitrate	16E04-B03-322132	1
Caelo	Miconazole nitrate	16144717	6
Fagron	Miconazole nitrate	16E04-B03-321367	1
Gehe	Miconazole nitrate	16144702	1
Fagron	Miconazole nitrate	16e04-b03-322131	2
Caesar & Loretz GmbH	Miconazole nitrate	16144717	1
Caelo	Miconazole nitrate	16144716	16
Caelo	Miconazole nitrate	16144711	8
Noweda	Miconazole nitrate	16144704	1
Fagron	Miconazole nitrate	1508-B07-314838	1
Fagron	Miconazole nitrate	16E04-B03-330082	6
Gehe	Miconazole nitrate	16E04-B03-327362	1
GEHE	Miconazole nitrate	16144716	1
Phoenix	Miconazole nitrate	15E04-B03-327367	1
Hedinger	Miconazole nitrate	16144720	2
Caelo	Miconazole nitrate	16e04b03327367	1
Anzag	Miconazole nitrate	16144716	1
Caelo	Miconazole nitrate	16144720	3
Euro OTC	Miconazole nitrate	1611024-015307	1
Sanacorp EK:5,95 EUR...	Miconazole nitrate	16144703	1
Euro OTC	Miconazole nitrate	1611024-015330	1
Euro OTC	Miconazole nitrate	1705039-01	5
phönix	Miconazole nitrate	16144716	1
Caelo	Miconazole nitrate	16144721	6
Euro OTC	Miconazole nitrate	16E04-B03-327362	2
Euro OTC	Miconazole nitrate	1705039-015371	1
Fagron	Miconazole nitrate	17C01-B02-334877	3
Caelo	Miconazole nitrate	16144726	9
Fagron	Miconazole nitrate	2900/09/16	3
Fagron	Miconazole nitrate	17C01-B02-225671	1
Bomastus / Alliance Hea...	Miconazole nitrate	16E04-B03-327367	1
Bombastus	Miconazole nitrate	16144725	1
Caelo	Miconazole nitrate	17217505	10
Euro OTC	Miconazole nitrate	1705039-015432	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Miconazole nitrate	1710020-01	6
Fagron	Miconazole nitrate	17C01-B02-335671	2
Caelo	Miconazole nitrate	16144725	9
Fagron	Miconazole nitrate	17c01-b02-335671	1
Euro OTC	Miconazole nitrate	1710020-015457	1
Phönix	Miconazole nitrate	17217502	1
Fagron	Miconazole nitrate	16E04-B03-332373	2
Kehr	Miconazole nitrate	17C01-B02-334877	1
Fagron	Miconazole nitrate	17C01-B02-340778	3
Fagron	Miconazole nitrate	17c01-b02-334877	1
Noweda	Miconazole nitrate	17217505	1
Caelo	Miconazole nitrate	17C01B02340778	1
Fagron	Miconazole nitrate	17C01-B02-334882	1
Caelo	Miconazole nitrate	17217502	9
Fagron	Miconazole nitrate	17C01-B02-341395	4
Sanacorp W.E:27.03.18 ...	Miconazole nitrate	16144726	2
Fagron	Miconazole nitrate	17c01-b02-340778	1
Fiebig	Miconazole nitrate	16144726	1
Fagron	Miconazole nitrate	18B06-B03-345419	4
PhoenixWE: 28.04.18 EK:...	Miconazole nitrate	17217505	1
Caelo	Miconazole nitrate	17217503	5
Fagron	Miconazole nitrate	18b06-b03-345423	1
euro AHD	Miconazole nitrate	1710020-015633	1
Caelo	Miconazole nitrate	18057903	3
euro AHD	Miconazole nitrate	1710020-015639	1
Fagron	Miconazole nitrate	18B06-B03-345423	1
Fagron	Miconazole nitrate	18C23-B02-347802	2
Fagron	Miconazole nitrate	18B06-B03-345422	1
Caelo	Miconazole nitrate	18057902	5
Fagron	Miconazole nitrate	18B06-B03-347788	2
Euro OTC	Miconazole nitrate	1803028-01	2
Fagron	Miconazole nitrate	18C23-B02-351310	1
Caelo	Miconazole nitrate	18057906	4
gehe-06.11.18	Miconazole nitrate	18057906	1
Caelo	Miconazole nitrate	18057912	3
Caelo	Miconazole nitrate	18057907	4
Caelo	Miconazole nitrate	18B06b0334778	1
Euro OTC	Miconazole nitrate	18057912	1
Fagron	Miconazole nitrate	18C23-B02-353243	1
Anzag	Miconazole nitrate	18C23-B02-353243	1
Caelo	Miconazole nitrate	18057914	1
Fagron	Miconazole nitrate	18C23-B02-350961	1

- 77 949 spectra from 565 *Apo-Ident* customers from a total of 25 895 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Miconazole nitrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Miconazole nitrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The

following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	294	0	74 202
Type B	0	807	1	126 084
Type C	0	950	30	77 949

The substance/substance group *Miconazole nitrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.9592 %)
Type B	100.0000 % (> 99.9901 %)	99.8762 % (> 99.5050 %)
Type C	100.0000 % (> 99.8817 %)	96.9388 % (> 96.6327 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20875	22630	5.22	177.58
21649	21350	7.09	175.68
21350	21350	0.00	177.15
21900	21900	0.00	178.75
22630	22630	0.00	177.82
20817	21350	3.66	176.44

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Minoxidil**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20879-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Minoxidil; Minoxidilum

Special notes

When selecting the *Minoxidil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Minoxidil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Minoxidil	13039501	20879	40	20130306
Caelo	Minoxidil	14093701	21359	40	20140428
Euro OTC	Minoxidil	1311038-01	21630	40	AR-15-FG-007848-01
Euro OTC	Minoxidil	1411006-01	21912	40	20141210
Euro OTC	Minoxidil	1509035	21933	40	20151016*
Euro OTC	Minoxidil	1602013	22365	40	20160225*
Euro OTC	Minoxidil	1612011	22982	40	20170130*

Validation samples

A total of 280317 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 *Minoxidil*. These samples are listed above in the [calibration samples](#) section.
- 74216 spectra from a total of 1616 batches from further 372 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 [†].

- 579 spectra of 15 reference samples from the substance/substance group *Minoxidil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Minoxidil	14093701	21361	40
Euro OTC	Minoxidil	1311038-01	21630 [†]	19
Euro OTC	Minoxidil	1411006-01	21912 [†]	20
Euro OTC	Minoxidil	1509035	21933 [†]	20
Euro OTC	Minoxidil	1602013	22365 [†]	20
Euro OTC	Minoxidil	1607007	22688	40
Euro OTC	Minoxidil	1705008	23437	40
Caelo	Minoxidil	172278	23816	40
Euro OTC	Minoxidil	1710043	23896	40
Euro OTC	Minoxidil	1803004	24062	40
Euro OTC	Minoxidil	1807018-01	24190	40
Euro OTC	Minoxidil	1411006-01	21912SI	60
Euro OTC	Minoxidil	1509035	21933SI	60
Euro OTC	Minoxidil	1602013	22365SI	60
Euro OTC	Minoxidil	1612011	22982SI	40

- 126313 spectra from a total of 2777 batches from further 781 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.

- 1075 spectra from 282 *Apo-Ident* customers from 288 batches from the substance/substance group *Minoxidil*.

Supplier	Substance	Batch	Spectra
Euro OTC	Minoxidil	1108039-01	1
Euro OTC	Minoxidil	1102010-02	1
Caelo	Minoxidil	11150209	1
Euro OTC	Minoxidil	1112024-02	5
Caelo	Minoxidil	11K11-n09	1
Caelo	Minoxidil	11e17-n07	1
Caelo	Minoxidil	11150207	1
Euro OTC	Minoxidil	1112024-03	3
Caelo	Minoxidil	11302003	1
Fagron	Minoxidil	11K11-N09	3
Phönix	Minoxidil	1112024-03	1
Fiebig ek: 36.06EUR 31.0812	Minoxidil	111202403	1
Fagron	Minoxidil	12A25-N04	4
Caelo	Minoxidil	12023902	1
Euro OTC	Minoxidil	1203035-01	10
Euro OTC	Minoxidil	1112024-01	1
Caelo	Minoxidil	11302005	1
Fagron	Minoxidil	4110I-02844	1
Fagron	Minoxidil	11E17-N07	1
Anzag 18.10.12 ek:40,14	Minoxidil	1203035-01	1
Anzag 14.11.12 ek:40,14	Minoxidil	120303501	1
Fagron	Minoxidil	612212844	1
Caelo	Minoxidil	12023901	2
Caelo	Minoxidil	1112024-01	1
Caelo	Minoxidil	12023907	4
Euro OTC	Minoxidil	1203035-03	11
Caelo	Minoxidil	20151112-5	1
Audor Pharma	Minoxidil	AP020/11M	3
Fagron	Minoxidil	12C29-N05	5
Caelo	Minoxidil	12H07-N03	4
EuRho	Minoxidil	1105030-02	1
Sanacorp	Minoxidil	1203035-01	1
Fagron	Minoxidil	12H07-N03	11
EuRho	Minoxidil	1108039-02	2
Caelo	Minoxidil	1203035	1
Euro OTC	Minoxidil	1203035-02	6
Anzag	Minoxidil	1112024-02	1
Euro OTC	Minoxidil	2002312844	1
Fagron	Minoxidil	120303503	1
Caelo	Minoxidil	12023908	1
Bombastus	Minoxidil	1112024-03	1
phönix	Minoxidil		1
Fagron	Minoxidil	12H07N03	1
Caelo	Minoxidil	12273704	3
A.H.D	Minoxidil	1210056-01	1
Sanacorp	Minoxidil	1210056-01	1
Euro OTC	Minoxidil	1210056-01	13

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Supplier	Substance	Batch	Spectra
Caelo	Minoxidil	1203035-01	1
Caelo	Minoxidil	12273703	2
Alliance Healthcare	Minoxidil	1210056-01	1
Europharm/Sanacorp	Minoxidil	1210056-01	1
EUro/AHD	Minoxidil	1203035-03	2
Euro OTC	Minoxidil	12100056-01	1
Alliance Healthc. 15.05...	Minoxidil	1203035-03	1
Caelo	Minoxidil	13039501	7
Caelo	Minoxidil	1210056-01	2
Caelo	Minoxidil	31051305	1
Fagron	Minoxidil	12H07-N03	1
Anzag	Minoxidil	13E13-N10	1
Euro OTC	Minoxidil	121005601	1
Audor Pharma	Minoxidil	AP010/12M	5
Fagron	Minoxidil	13E13-N10	8
Caelo	Minoxidil	1309501	1
AHD	Minoxidil	1210056-01	1
Fagron	Minoxidil	13H07-N03	1
Euro OTC	Minoxidil	1210056-02	25
Sanacorp	Minoxidil	120056-01	1
Fagron	Minoxidil	12H07-N030265/432	1
Fagron	Minoxidil	12C29-N050087/240	1
Fagron	Minoxidil	12H07-No3	1
Euro OTC	Minoxidil	1108039-03	1
Caelo	Minoxidil	1210056-02	3
Doppeleiche Apotheke	Minoxidil	13E13-N10	2
Caelo	Minoxidil	13039503	3
Alliance Healthcare	Minoxidil	1210056-02	1
Caesar & Loretz GmbH	Minoxidil	13039501	1
Sanacorp	Minoxidil	1210056-02	2
Fagron	Minoxidil	27081301	1
ICROM	Minoxidil	6/12	1
AHC 14.08.13 EK40,14	Minoxidil	1210056-02	1
Euro OTC	Minoxidil	6/12	2
Caelo	Minoxidil	3013M-02844	1
Euro OTC	Minoxidil	1304029-01	16
Fagron	Minoxidil	1210056-02	1
Caelo	Minoxidil	13179501	2
Caelo	Minoxidil	13E13-N10	1
euroct/Gehe	Minoxidil	1304029-01	1
Phönix	Minoxidil	1304029-01	1
Euro/Gehe	Minoxidil	1112024-03	1
Caelo	Minoxidil	13179504	2
Sanacorp	Minoxidil	13179502	2
Euro OTC	Minoxidil	1203035	1
Caelo	Minoxidil	12273710	1
Caelo	Minoxidil	13179503	6
Sanacorp	Minoxidil	13179501	2
Euro OTC	Minoxidil	1009042-01	3
EuRho / Noweda	Minoxidil	1304029-02	1
Euro OTC	Minoxidil	13001	1
Fagron	Minoxidil	13E13N10	1
Fagron	Minoxidil	12H07-N03	1
Fagron	Minoxidil	26111302	1
Euro OTC	Minoxidil	1304029-02	15
Sanacorp	Minoxidil	1304029-02	3
Euro OTC	Minoxidil	4/13	2
Hedinger/Sanacorp	Minoxidil	12C29-N05	1
Fagron	Minoxidil	12C29-N050145/240	1
Gehe	Minoxidil	AP006/13M	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Minoxidil	130402902	1
Caelo	Minoxidil	13179502	5
Caelo	Minoxidil	13179501-3467312121	1
Euro	Minoxidil	1304029-02	1
Fagron	Minoxidil	13I23-N07	6
Euro OTC	Minoxidil	130402901	1
Caelo	Minoxidil	130402902	1
Euro OTC	Minoxidil	1304029-C2	1
Bombastus	Minoxidil	4/13	1
Phönix	Minoxidil	1203035-02	1
Fagron	Minoxidil	11021402	1
Caelo	Minoxidil	13/23-N07	1
Caelo	Minoxidil	130402901	1
Euro OTC	Minoxidil	1311038-01	29
Fagron	Minoxidil	13J29-B02	1
Euro OTC	Minoxidil	10/13	1
Caelo	Minoxidil	22031402	1
Euro OTC	Minoxidil	104029-02	1
Audor Pharma	Minoxidil	AP006/13M	2
Fagron	Minoxidil	13J23N07	2
PhOENIX 19.03.2012	Minoxidil	1311038-01	2
Caelo	Minoxidil	1311038-01	2
Euro OTC	Minoxidil	131103801	4
Fagron	Minoxidil	13I23-N07	1
Euro OTC	Minoxidil	120303503	1
Fagron	Minoxidil	13K04-B05-290377	5
Vdl 14.07.14	Minoxidil	1311038-01	1
AHD	Minoxidil	1311038-01	1
Caelo	Minoxidil	13373106	1
Audor Pharma	Minoxidil	414E-02844	1
Euro OTC	Minoxidil	29071402	1
Hedinger	Minoxidil	14B04-B07	2
Euro OTC	Minoxidil	140502801	3
Sanacorp	Minoxidil	14093701	1
Ichthyol-Gesellschaft	Minoxidil	1311038-01	1
Caelo	Minoxidil	13I23-N07	2
Euro OTC	Minoxidil	1405028-01	29
Caelo	Minoxidil	14093707	1
Fagron	Minoxidil	1311038-01	1
sanacorp	Minoxidil	1405028-01	1
Caelo	Minoxidil	14093703	3
Euro OTC	Minoxidil	700158	1
icrom spa	Minoxidil	511v	1
Fagron	Minoxidil	13K04-B05-290379	2
Caelo	Minoxidil	13K04B05290380	1
Euro OTC	Minoxidil	13110838-01	1
Euro OTC	Minoxidil	14050281	1
sanacorp	Minoxidil	13K04-B05-290379	1
Fagron	Minoxidil	7/13	1
Euro/ Phönix	Minoxidil	1405028-01	1
Gehe	Minoxidil	1405028-01	1
Sanacorp	Minoxidil	1405028-01	1
Fagron	Minoxidil	13K04-B05-290380	3
Fagron	Minoxidil	14B04-B07	1
Fagron	Minoxidil	14B04-B07-290883	3
Noweda	Minoxidil	14093703	1
Euro OTC	Minoxidil		3
Euro/Gehe	Minoxidil	140528-01	1
Fagron	Minoxidil	13K04-B05-0004	1
Sanacorp	Minoxidil	14093702	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Minoxidil	1405028-1	1
Caelo	Minoxidil	14093702	2
Euro OTC	Minoxidil	140528-01	1
Sanacorp	Minoxidil	140502801	1
Caelo	Minoxidil	1405028-01	1
Audor Pharma	Minoxidil	AP088/14M	1
Caelo	Minoxidil	14093706	3
Caelo	Minoxidil	1411006-01	2
Euro OTC	Minoxidil	1411006-01	37
Caelo	Minoxidil	14234505	5
Alliance health	Minoxidil	1411006-01	3
EuRho/Fiebig	Minoxidil	1411006-01	1
Fagron	Minoxidil	14B04-B07-297364	1
Audor Pharma	Minoxidil	AP008/14M	6
Fagron	Minoxidil	14L03-B02-301541	1
Caelo	Minoxidil	14234502	2
Caelo	Minoxidil	14L03-B02-301431	1
Euro OTC	Minoxidil	141100601	5
Fagron	Minoxidil	14L03-B02-301430	2
Fagron	Minoxidil	1411006-01	1
Caelo	Minoxidil	2905047-01	1
Anzag	Minoxidil	14234505	1
Euro OTC	Minoxidil	1411006601	1
Fagron	Minoxidil	14L03-B02-301429	6
Audor Pharma	Minoxidil	8/14M	1
Caelo	Minoxidil	14234509	3
Fagron	Minoxidil	1420001962	1
VDL;81,0EUR;21.05.15	Minoxidil	1411006-01	1
Euro OTC	Minoxidil	6614849	1
Fagron	Minoxidil	15E19-B06	1
Sanacorp	Minoxidil	1411006-01	1
Euro OTC	Minoxidil	1504013-01	29
Caelo	Minoxidil	5081502	1
Sanacorp	Minoxidil	1504013-01	1
Fagron	Minoxidil	14L03-Bo2-301430	1
Fagron	Minoxidil	15E19-B06-308182	6
Audor Pharma	Minoxidil	AP007/15M	4
Caelo	Minoxidil	1504013-01	5
Fagron	Minoxidil	14L03-B02301434	1
Caelo	Minoxidil	150401301	1
Fagron	Minoxidil	14L03-B02-301431	1
Fagron	Minoxidil	14L03-B02301429	1
Euro OTC	Minoxidil	150401-01	1
Euro OTC	Minoxidil	1504013-02	24
Fagron	Minoxidil	15F02-B08	1
Fagron	Minoxidil	1520000768	2
Fagron	Minoxidil	14L03-B02-30129	1
Caelo	Minoxidil	15E19-B06-308183	1
Fagron	Minoxidil	14L03-B02	2
Fagron	Minoxidil	15E19-B06-308183	5
Caelo	Minoxidil	15230804	4
Audor Pharma	Minoxidil	AP016/15M	6
Caelo	Minoxidil	15230802	3
anzag	Minoxidil	1504013-02	1
Fagron	Minoxidil	15E19-B06-308181	2
Euro OTC	Minoxidil	1509035-01	28
Euro OTC	Minoxidil	1504013-2	1
Fagron	Minoxidil	15e19-b06-308180	1
Caelo	Minoxidil	17011602	1
Fagron	Minoxidil	15E19-06-308183	1

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Supplier	Substance	Batch	Spectra
Fagron	Minoxidil	15E19-B06-308180	5
Fagron	Minoxidil	15E19-B06-308183	1
Caelo	Minoxidil	20160211-1	1
AHD	Minoxidil	1504013-02	1
Caelo	Minoxidil	1509035-01	3
Euro	Minoxidil	1504013-01	2
phönix	Minoxidil	1509035-01	1
Fagron	Minoxidil	15F02-B09-312663	2
Caelo	Minoxidil	15230805	2
Fagron	Minoxidil	15E19-B09-308181	1
Caelo	Minoxidil	15E19-B06-309180	1
Euro OTC	Minoxidil	1602013-01	30
Caelo	Minoxidil	15230803	3
Caelo	Minoxidil	1602013-01	6
Caelo	Minoxidil	1509035	1
Audor Pharma	Minoxidil	AP-016/15M	1
Euro/Anzag	Minoxidil	150903501	1
Gehe/Euro	Minoxidil	150903501	1
Caelo	Minoxidil	15230811	4
Audor Pharma	Minoxidil	AP001/16M	7
phönix	Minoxidil	1602013-01	3
Fagron	Minoxidil	15K17-B05-318241	1
Caelo	Minoxidil	160013-01	1
Gehe	Minoxidil	1602013-01	1
Euro OTC	Minoxidil	1602013-1	1
Fagron	Minoxidil	15H07-B01-314726	1
Fagron	Minoxidil	15K17-B05-318240	1
Phoenix	Minoxidil	1602013-02	1
Euro OTC	Minoxidil	1602013-02	10
Caelo	Minoxidil	1602013-02	3
Caelo	Minoxidil	15K17-B05-318240	1
Caelo	Minoxidil	15436202	6
Caelo	Minoxidil	160201302	1
Fagron	Minoxidil	15K17-B05-320188	3
Euro OTC	Minoxidil	1607007-01	23
Fagron	Minoxidil	15K17-B05-318691	2
Caelo	Minoxidil		3
Fagron	Minoxidil	15K197-B05-318411	1
Euro/Noweda	Minoxidil	1602013-02	1
Caelo	Minoxidil	15436201	4
Euro OTC	Minoxidil	1602016-01	1
Caelo	Minoxidil	15K17-B06-321926	1
Icrom/Gehe	Minoxidil	1602013-01	1
Fagron	Minoxidil	1520002631	1
Caelo	Minoxidil	121005601	1
Euro OTC	Minoxidil	16070007-01	1
Phönix	Minoxidil	1602013-02	1
Caelo	Minoxidil	15436204	2
Fagron	Minoxidil	15K17-B05-318411	1
Caelo	Minoxidil	1607007-01	2
apo-ident.	Minoxidil	1607007-07	1
Fagrin	Minoxidil	15K17-B06-321926	1
Fagron	Minoxidil	15K17-B06-321926	5
Caelo	Minoxidil	160707-01	1
Caelo	Minoxidil	15K17-B05-318692	1
Fagron	Minoxidil	15K17-B06-324965	2
Fagron	Minoxidil	15K17-B06-321927	2
Caelo	Minoxidil	AP011/16M	1
Fagron	Minoxidil	15K17-B06-325490	1
Fagron	Minoxidil	15E19-B06-308179	1

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Supplier	Substance	Batch	Spectra
Fagron	Minoxidil	15K17-B06-321928	2
Sanacorp, 81,00EUR, 27.1.17	Minoxidil	1607007-01	1
Audor Pharma	Minoxidil	AP011/16M	1
Euro OTC	Minoxidil	1607007	1
Caelo	Minoxidil	15436202/1060217	1
Caelo	Minoxidil	1520002455	1
Fagron	Minoxidil	321926	1
Euro OTC	Minoxidil	1612011-01	34
Caelo	Minoxidil	15436404	3
Audor Pharma	Minoxidil	AP012/16M	4
Caelo	Minoxidil	13179507	3
Gehe	Minoxidil	15436406	1
Euro OTC	Minoxidil	1607001-01	1
Euro/Phönix	Minoxidil	161201101	2
Audor Pharma	Minoxidil	AP006/17M	2
Gehe	Minoxidil	15436201	1
Noweda/Apomix	Minoxidil	1504013-02	1
Fagron	Minoxidil	15K17-B06	1
Phönix	Minoxidil	1612011-01	1
Euro OTC	Minoxidil	12/16	1
EuRho/Noweda	Minoxidil	1607007-01	1
Caelo	Minoxidil	15k17-b06-324965	1
Euro OTC	Minoxidil	1612011	1
Caelo	Minoxidil	15H07-B03-317340	1
Euro OTC	Minoxidil	19/16	1
Audor Pharma	Minoxidil	AP012/16M/5270	1
phönix	Minoxidil	1612011-01	2
Gehe	Minoxidil	1612011-01	1
Noweda/ Infecto Pharm	Minoxidil	1607007-01	1
Fagron	Minoxidil	15K17-B06-325491	2
Caelo	Minoxidil	15436406	3
Fagron	Minoxidil	1612011-01	1
Audor Pharma	Minoxidil		20
Euro OTC	Minoxidil	170703M/1602013-02	1
Fagron	Minoxidil	16J24-B04-328218	2
Fagron	Minoxidil	17B22-B01-334447	1
Fagron	Minoxidil	16J24-B04-328226	3
Fagron	Minoxidil	15436408	1
Sanacorp	Minoxidil	1612011-01	1
Fagron	Minoxidil	2/16M	2
Fagron	Minoxidil	17B22-B01	2
Euro OTC	Minoxidil	1705008-01	21
Euro OTC	Minoxidil	1919	1
Fagron	Minoxidil	1/16M	1
Euro OTC	Minoxidil	2091714	1
Euro/Noweda	Minoxidil	1612011-01	1
Hedinger/Fiebig	Minoxidil	1612011-01	1
Caelo	Minoxidil	15436412	1
Caelo	Minoxidil	15436414	3
Caelo	Minoxidil	16J24-B05-331128	1
Fagron	Minoxidil	16J24-B05	1
Phönix	Minoxidil	1705008-01	1
Caelo	Minoxidil	1705008-01	2
Caelo	Minoxidil	AP006/17M	1
Caelo	Minoxidil	15436408	2
Caelo	Minoxidil	170500801	2
Fagron	Minoxidil	17B22-B01-335427	2
Caelo	Minoxidil	15230812	1
Euro OTC	Minoxidil	12/17	1
Fagron	Minoxidil	17B22-B02-336690	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Minoxidil	170500801	2
Phönix /euro	Minoxidil	170500801	2
Fagron	Minoxidil	1705008-01	1
Euro OTC	Minoxidil	1710043-01	17
EuRho/ Alliance	Minoxidil	1705008-01	1
Fagron	Minoxidil	17B22-B02-336689	2
Caelo	Minoxidil	5217M-02844	1
Euro OTC	Minoxidil	16120-01	1
Fagron	Minoxidil	17B22-B02	1
Euro OTC	Minoxidil	171004301	3
Caelo	Minoxidil	16J24-B05-332092	1
Fagron	Minoxidil	17B22/B02/336689	2
Caelo	Minoxidil	15436415	1
Caelo	Minoxidil	K0071/16/04/065	1
Gehe	Minoxidil	1710043-01	1
Ichthyol/Noweda	Minoxidil	17117803	1
Euro OTC	Minoxidil	17050008	1
Caelo	Minoxidil	1070318/17227803	1
Caelo	Minoxidil	1710043-01	2
Fagron	Minoxidil	16J24-B05-332092	2
Fagron	Minoxidil	17H08-B06	1
EuRho/Noweda	Minoxidil	1710043-01	2
Kehr	Minoxidil	1705008-01	1
Euro OT/Phönix	Minoxidil	1710043-01	1
Caelo	Minoxidil	17227801	6
Audor Pharma	Minoxidil	APK007	1
Euro OTC	Minoxidil	17H08-B06	1
Caelo	Minoxidil	17227803	2
EuRho/Kehr	Minoxidil	30/17	1
Fagron	Minoxidil	17H08-B06-341376	3
Fagron	Minoxidil	17H08-B06-341377	3
Caelo	Minoxidil	14062018-RQ-A	1
europarm/gehe	Minoxidil	1710043-01	1
Euro OTC	Minoxidil	17100-43-01	1
Euro OTC	Minoxidil	1803004-01	2
Fagron	Minoxidil	16J24-B04-329291	1
Euro OTC	Minoxidil	15081829	1
Caelo	Minoxidil	1807018-01	3
Jenne	Minoxidil	17H08-B06-341377	1
Euro OTC	Minoxidil	1707018-01	1
Fagron	Minoxidil	18C19-B01-348985	1
Caelo	Minoxidil	1803004-01	1
Euro OTC	Minoxidil	1807018	1
Fagron	Minoxidil	18C20-B01	1
Euro OTC	Minoxidil	1807018-01	6
Fagron	Minoxidil	18C19-B01-348984	1
Fagron	Minoxidil	18C20-B01-351844	1
Caelo	Minoxidil	180701801	1
Fagron	Minoxidil	18C20-B01-352116	1
Fagron	Minoxidil	18C20-B01-352629	1
Kehr	Minoxidil	1803004-01	1

- 77 854 spectra from 565 *Apo-Ident* customers from a total of 25 855 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Minoxidil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Minoxidil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	252	28	74 216
Type B	0	563	16	126 313
Type C	0	1063	12	77 854

The substance/substance group *Minoxidil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	90.0000 % (> 88.9286 %)
Type B	100.0000 % (> 99.9901 %)	97.2366 % (> 96.7185 %)
Type C	100.0000 % (> 99.8817 %)	98.8837 % (> 98.6047 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20879	21630	4.95	40.25
21359	21630	4.63	39.60
21630	21630	0.00	41.06
21912	21933	3.59	38.05
21933	21933	0.00	34.17
22365	22365	0.00	41.04
22982	22982	0.00	42.83

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Mometasone furoate, micronized
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20100-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mometasone furoate, micronized; Mometasoni furoas micronisatum

Special notes

When selecting the *Mometasone furoate, micronized* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Mometasone furoate, micronized*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Mometasone furoa...	13F17-N01	20850	40	20130620
Euro OTC	Mometasone furoa...	1403015-01	21602	40	20140503
Euro OTC	Mometasone furoa...	1510036	22238	40	20151118*
Caelo	Mometasone furoa...	160286	22433	40	20160316*
Fagron	Mometasone furoa...	16A20-B06-319750	22887	40	20160209

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Mometasone furoa...	1610009	23136	40	20170321*
Fagron	Mometasone furoa...	13F17-N01	20850SI	29	20130620
Euro OTC	Mometasone furoa...	1403015-01	21602SI	21	20140503
Euro OTC	Mometasone furoa...	1510036	22238SI	20	20151118*
Fagron	Mometasone furoa...	16A20-B06-319750	22887SI	30	20160209

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 340 spectra of 10 reference samples from the substance/substance group *Mometasone furoate, micronized*. These samples are listed above in the [calibration samples](#) section.
- 74 156 spectra from a total of 1617 batches from further 372 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 [†].

- 506 spectra of 18 reference samples from the substance/substance group *Mometasone furoate, micronized*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mometasone furoate, micronized	13304605	21374	60
Euro OTC	Mometasone furoate, micronized	1403015-01	21602 [†]	20
Euro OTC	Mometasone furoate, micronized	1510036	22238 [†]	20
Caelo	Mometasone furoate, micronized	160286	22433 [†]	20
Euro OTC	Mometasone furoate, micronized	1606021	22715	40
Caelo	Mometasone furoate, micronized	163532	23046	40
Euro OTC	Mometasone furoate, micronized	1711027	23878	40
Euro OTC	Mometasone furoate, micronized	1810008	24295	40
Fagron	Mometasone furoate, micronized	13F17-N01	20850SI [†]	15
Caelo	Mometasone furoate, micronized	13304605	21374SI	38
Euro OTC	Mometasone furoate, micronized	1403015-01	21602SI [†]	10
Euro OTC	Mometasone furoate, micronized	1510036	22238SI [†]	10
Caelo	Mometasone furoate, micronized	160286	22433SI	30

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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	Mometasone furoate, micronized	1606021	22715SI	33
Caelo	Mometasone furoate, micronized	163532	23046SI	23
Euro OTC	Mometasone furoate, micronized	1610009	23136SI	20
Euro OTC	Mometasone furoate, micronized	1711027	23878SI	27
Euro OTC	Mometasone furoate, micronized	1810008	24295SI	20

- 126386 spectra from a total of 2779 batches from further 781 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.

- 597 spectra from 222 *Apo-Ident* customers from 227 batches from the substance/substance group *Mometasone furoate, micronized*.

Supplier	Substance	Batch	Spectra
Fagron	Mometasone furoate, micronized	11F08-N03	1
Fagron	Mometasone furoate, micronized	11C02-N03	2
Fagron	Mometasone furoate, micronized	11K28-N09	1
Fagron	Mometasone furoate, micronized	11h10-n04	1
Caelo	Mometasone furoate, micronized		1
Caelo	Mometasone furoate, micronized	12035601	1
Fagron	Mometasone furoate, micronized	12J29-N03	4
Fagron	Mometasone furoate, micronized	12H09-N02	7
Caesar & Loretz GmbH	Mometasone furoate, micronized	12035601	1
Fagron	Mometasone furoate, micronized	12J29-N01	1
Caelo	Mometasone furoate, micronized	12035608	1
Anzag	Mometasone furoate, micronized	12J29N03	1
Caelo	Mometasone furoate, micronized	12351201	1
Fagron	Mometasone furoate, micronized	12I29-N03	1
Euro OTC	Mometasone furoate, micronized	1203024-02	1
Fagron	Mometasone furoate, micronized	12e02-n11	1
Fagron	Mometasone furoate, micronized	11H10-N01	1
Fagron	Mometasone furoate, micronized	12B22-N04	1
Fagron	Mometasone furoate, micronized	13D08-N06	12
Caelo	Mometasone furoate, micronized	12351205	1
Fagron	Mometasone furoate, micronized	12E02-N11	2
Anzag	Mometasone furoate, micronized	13D08-N06	1
Fagron	Mometasone furoate, micronized	13F7-N01	1
Gehe	Mometasone furoate, micronized	13D08-N06	1
Fagron	Mometasone furoate, micronized	12B22-N01	1
Holdermann	Mometasone furoate, micronized	13D08-N06	1
Fagron	Mometasone furoate, micronized	10C29-N10	1
Fagron	Mometasone furoate, micronized	13D08N06	1
Caelo	Mometasone furoate, micronized	240913a	1
Caelo	Mometasone furoate, micronized	13F27-N02	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	Mometasone furoate, micronized	13F17-N01	7
Fagron	Mometasone furoate, micronized	13F27-N02	6
Caelo	Mometasone furoate, micronized	12035607	2
Fagron	Mometasone furoate, micronized	13H13-N04	1
Fagron	Mometasone furoate, micronized	10805-N12	1
Fagron	Mometasone furoate, micronized	13d08-n06	1
Phönix	Mometasone furoate, micronized	13D08-N06	1
Caelo	Mometasone furoate, micronized	18102013B	1
Fargon	Mometasone furoate, micronized	13H13-N04	1
Fagron	Mometasone furoate, micronized	13f17-n01	1
Caelo	Mometasone furoate, micronized	12351207	1
Caelo	Mometasone furoate, micronized	13H13-N04	1
Fagron	Mometasone furoate, micronized	13H13-N04	8
Gehe	Mometasone furoate, micronized	13H13-N04	2
Phönix	Mometasone furoate, micronized	13/23-N02	1
Caelo	Mometasone furoate, micronized	13J23-N02	2
Caelo	Mometasone furoate, micronized	12339604	1
Fagron	Mometasone furoate, micronized	13J23-N02	13
Caelo	Mometasone furoate, micronized	NT1568M	1
Alliance Health 27.01.2...	Mometasone furoate, micronized	13J23-N02	1
Caelo	Mometasone furoate, micronized	12351215	2
EuRho/Phönix	Mometasone furoate, micronized	1307037-01	2
Euro OTC	Mometasone furoate, micronized	1307037-01	1
GEHE 17.04.2014	Mometasone furoate, micronized	13J23-N02	1
Fagron	Mometasone furoate, micronized	1814E3640	1
Fagron	Mometasone furoate, micronized	13j23-N02	1
Fagron	Mometasone furoate, micronized	NT1568M	3
Caelo	Mometasone furoate, micronized	14C07-B05-291268	8
Fagron	Mometasone furoate, micronized	2114M3640	1
Phoenix	Mometasone furoate, micronized	14C07-B05-291268	1
Fagron	Mometasone furoate, micronized	14C07-B05-291268	3
Fagron	Mometasone furoate, micronized	13j23-no2	1
Caelo	Mometasone furoate, micronized	13304604	1
Fagron	Mometasone furoate, micronized	3313A-07030	1
AHD 20.06.14 EK 37,29	Mometasone furoate, micronized	12C07-B05-291268	1
Fagron	Mometasone furoate, micronized	14C07-B05-291266	2
Phönix Gotha	Mometasone furoate, micronized	1403015-01	1
Fagron	Mometasone furoate, micronized	NS1513M	1
Fagron	Mometasone furoate, micronized	14E20-B04-291265	3
Holdermann	Mometasone furoate, micronized	14C07-B05-29126	1
Caelo	Mometasone furoate, micronized	14E20-B04	1
Caelo	Mometasone furoate, micronized	701834-0002	1
Fagron	Mometasone furoate, micronized	14E20-B04-294645	5
Caelo	Mometasone furoate, micronized	12351202	1
Caelo	Mometasone furoate, micronized	13304605	1
Fagron	Mometasone furoate, micronized	14E20-B04-291267	2
Fagron	Mometasone furoate, micronized	14e20b04291265	1
Fagron	Mometasone furoate, micronized	14C07-B05-291264	1
Euro OTG	Mometasone furoate, micronized	1403015-01	1
Euro OTC	Mometasone furoate, micronized	1408010-01	1
Fagron	Mometasone furoate, micronized	14e20-b04-291265	1
Fagron	Mometasone furoate, micronized	14E20-B04	2
Caelo	Mometasone furoate, micronized	N01352M	1
Fagron	Mometasone furoate, micronized	14H06-B07297240	1
Caelo	Mometasone furoate, micronized	14H06-B07298481	1
Caelo	Mometasone furoate, micronized	NU0698M	1
Caelo	Mometasone furoate, micronized	14E20-B04-291267	1
Caelo	Mometasone furoate, micronized	13304606	1
Fagron	Mometasone furoate, micronized	14H06-B07-298482	7
Fagron	Mometasone furoate, micronized	14H06-B07-298481	2

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Supplier	Substance	Batch	Spectra
EuRho	Mometasone furoate, micronized	1408010-01	1
Caelo	Mometasone furoate, micronized	200315A	1
Caelo	Mometasone furoate, micronized	14281102	3
Fagron	Mometasone furoate, micronized	14H06-B07-297240	1
Fargon	Mometasone furoate, micronized	14h06-b07-298481	1
Caelo	Mometasone furoate, micronized	14281101	2
Caelo	Mometasone furoate, micronized	14281103	1
Fagron	Mometasone furoate, micronized	2714U-07030	1
Fagron	Mometasone furoate, micronized	14H06-B07-302376	2
Fagron	Mometasone furoate, micronized	15B11-B03-304122	5
Euro OTC	Mometasone furoate, micronized	1504012-01	6
Caelo	Mometasone furoate, micronized	15B11-B03-304121	2
Fagron	Mometasone furoate, micronized	15B11-B03-304121	5
Caelo	Mometasone furoate, micronized	15b11b03	1
Caelo	Mometasone furoate, micronized	15110305	3
Fagron	Mometasone furoate, micronized	15B11B03304122	1
Fagron	Mometasone furoate, micronized	15B11-B03-304120	6
Fagron	Mometasone furoate, micronized	14E20-B04-302374	2
Fagron	Mometasone furoate, micronized	15B11-B03-304124	1
Fagron	Mometasone furoate, micronized	15B11-B03-304123	12
Caelo	Mometasone furoate, micronized	15189802	1
Fagron	Mometasone furoate, micronized	15B11-B03	2
Fagron	Mometasone furoate, micronized	15b11-b03-308276	1
Caelo	Mometasone furoate, micronized	15B11B03304122	1
Sanacorp	Mometasone furoate, micronized	15189801	1
Fagron	Mometasone furoate, micronized	15G08-B11-310864	6
Fagron	Mometasone furoate, micronized	15B11-B03-308276	1
Fagron	Mometasone furoate, micronized	15G-B11-310864	1
Fagron	Mometasone furoate, micronized	15G08-B11-312233	3
Euro OTC	Mometasone furoate, micronized	1510036-01	8
Fagron	Mometasone furoate, micronized	15/11-B02-314479	5
Caelo	Mometasone furoate, micronized	15189801	1
Caelo	Mometasone furoate, micronized	15189807	3
Euro OTC	Mometasone furoate, micronized	1504012-02	1
Caelo/Noweda	Mometasone furoate, micronized	15279003	1
Cael Sanacorp 05.02.2016	Mometasone furoate, micronized	14H06-B07-298481	1
Fagron	Mometasone furoate, micronized	15/11-B02-315705	2
Fagron	Mometasone furoate, micronized	15I11-B02-314479	4
Fagron	Mometasone furoate, micronized	15/11-B02	4
Caelo	Mometasone furoate, micronized	1510036-001	1
Fagro	Mometasone furoate, micronized	1511B02	1
Fagron	Mometasone furoate, micronized	NU2504M	1
Fagron	Mometasone furoate, micronized	10E31-N26	1
Fagron	Mometasone furoate, micronized	15G08-B11-317182	7
Fagron	Mometasone furoate, micronized	5/0715	1
Fagron	Mometasone furoate, micronized	15G08-B11-0002	1
EuRho	Mometasone furoate, micronized	15/11-B02-315705	1
Caelo	Mometasone furoate, micronized	16028606	5
Fagron	Mometasone furoate, micronized	14H06-B07-302375	2
Caelo	Mometasone furoate, micronized	15189809	2
Caelo	Mometasone furoate, micronized	15/11-Bo2-314479	1
Caelo	Mometasone furoate, micronized	15279004	2
Fagron	Mometasone furoate, micronized	15G08-B11	2
Fagron	Mometasone furoate, micronized	15J11-B02-315705	1
Caelo	Mometasone furoate, micronized	15189804	1
Caelo	Mometasone furoate, micronized	NV1000M	1
Fagron	Mometasone furoate, micronized	2215I-07030	1
Fagron	Mometasone furoate, micronized	11H10-N04	1
Fagron	Mometasone furoate, micronized	15/11-B02-316705	1
Caelo	Mometasone furoate, micronized	16028601	2

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Supplier	Substance	Batch	Spectra
Fagron	Mometasone furoate, micronized	15B11-B03-308860	2
Caelo	Mometasone furoate, micronized	15G08-B11-317182	1
Fagron	Mometasone furoate, micronized	MOM008/0915	1
Caelo	Mometasone furoate, micronized	16028609	3
phönix	Mometasone furoate, micronized	15B11-b03	1
Fagron	Mometasone furoate, micronized	15B11B03308860	1
Caelo	Mometasone furoate, micronized	16028602	4
Fagron	Mometasone furoate, micronized	15B11B03304121	1
Fagron	Mometasone furoate, micronized	16A20-B06-319749	4
Fagron	Mometasone furoate, micronized	13Do8-N06	1
Caelo	Mometasone furoate, micronized	15G08-B11-310864	2
Caesar&lorenz,AHC,08.08...	Mometasone furoate, micronized		1
Fagron	Mometasone furoate, micronized	16A20-B06-319748	4
Euro OTC	Mometasone furoate, micronized	15G08-B11-317182	1
Euro OTC	Mometasone furoate, micronized	160602101	1
Fagron	Mometasone furoate, micronized	16A20-B06	3
Caelo	Mometasone furoate, micronized	15/11-B02-314479	1
Fagron	Mometasone furoate, micronized	16A20-B06319749	1
Caelo	Mometasone furoate, micronized	16A20-B06-319748	1
Caelo	Mometasone furoate, micronized	16028607	5
Euro OTC	Mometasone furoate, micronized	1606021-01	3
Fagron	Mometasone furoate, micronized	140305MF	1
Fagron	Mometasone furoate, micronized	16A20-B06-322739	4
Caelo	Mometasone furoate, micronized	16A20-B06-319749	1
Fagron	Mometasone furoate, micronized	15G08-B11-322737	3
Caesar u Loretz	Mometasone furoate, micronized	15279004	1
Fagron	Mometasone furoate, micronized	15G08-B11-322738	3
Fagron	Mometasone furoate, micronized	15G08B11322738	1
Fagron	Mometasone furoate, micronized	16C24-B03-324852	4
Fagron	Mometasone furoate, micronized	15G08	1
Caelo	Mometasone furoate, micronized	16028603	1
Caelo	Mometasone furoate, micronized	15G08-B11-322739	1
Fagron	Mometasone furoate, micronized	16A20-B06-319740	1
Caelo	Mometasone furoate, micronized	16C24-B03-324852	1
Alte Apotheke	Mometasone furoate, micronized	1606021-01	1
Caelo	Mometasone furoate, micronized	16C24B03324852	2
caesar&Loretz GmbH,Phön...	Mometasone furoate, micronized	16028604	1
Caelo	Mometasone furoate, micronized	16181708	2
Fagron	Mometasone furoate, micronized	16C24-B03-327346	4
Caelo	Mometasone furoate, micronized	16028604	2
Fragon/Sanacorp	Mometasone furoate, micronized	16C24-B03-324851	1
Phönix	Mometasone furoate, micronized	15G08-B11-322737	1
SanacorpWE:12.01.2017 ...	Mometasone furoate, micronized	16028602	1
Fagron	Mometasone furoate, micronized	16C24-B03	2
Caelo	Mometasone furoate, micronized	16028605	2
Fargon	Mometasone furoate, micronized	16C24-B03-324852	1
Fagron	Mometasone furoate, micronized	16C24-B03-324851	1
Caelo	Mometasone furoate, micronized	16181709	1
Phönix	Mometasone furoate, micronized	16c24-b03-327346	1
Fagron	Mometasone furoate, micronized	16j24-b11-329817	1
Fagron	Mometasone furoate, micronized	16C24	1
Fagron	Mometasone furoate, micronized	16C24-B03-326790	4
Caelo	Mometasone furoate, micronized	16181704	4
Fagron	Mometasone furoate, micronized	16J24-B11-329817	3
Caelo	Mometasone furoate, micronized	16181705	3
Gehe	Mometasone furoate, micronized	16353201	1
Caelo	Mometasone furoate, micronized	16181710	1
Caelo	Mometasone furoate, micronized	16181714	1
Caelo	Mometasone furoate, micronized	16353201	4
Fagron	Mometasone furoate, micronized	16C24-B03-327372	4

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Supplier	Substance	Batch	Spectra
Caelo	Mometasone furoate, micronized	16J24-B11-330978	1
Fagron	Mometasone furoate, micronized	16C24B03	1
Euro OTC	Mometasone furoate, micronized	15G08-B11-322738	2
Fagron	Mometasone furoate, micronized	16J24-B11-330978	4
Fagron	Mometasone furoate, micronized	16C24-B03-328272	4
Finteler Apotheke	Mometasone furoate, micronized	16028604	1
Caelo	Mometasone furoate, micronized	16181715	5
Euro OTC	Mometasone furoate, micronized	5991	1
Fagron	Mometasone furoate, micronized	16J24-B11-332112	5
Fagron	Mometasone furoate, micronized	16724-B11-332112	1
Caelo	Mometasone furoate, micronized	16028614	1
Fagron	Mometasone furoate, micronized	16J24-B11	3
Fagron	Mometasone furoate, micronized	16/24-B11-332122	1
Fagron	Mometasone furoate, micronized	16C24-b03-327372	1
Caelo	Mometasone furoate, micronized	16353204	2
Euro OTC	Mometasone furoate, micronized	1610009-01	9
Fagon	Mometasone furoate, micronized	16C24-B03	1
Caelo	Mometasone furoate, micronized	16J24-B11-332112	1
Audor Pharma	Mometasone furoate, micronized	APMOM006/0117M	2
Noweda	Mometasone furoate, micronized	16C24-B03-328272	1
Caelo	Mometasone furoate, micronized	16353205	2
Caelo	Mometasone furoate, micronized	16353207	9
Fagron	Mometasone furoate, micronized	16j24-b11	1
Finteler Apotheke	Mometasone furoate, micronized	16028603	1
Caelo	Mometasone furoate, micronized	16353206	3
Fagron	Mometasone furoate, micronized	16J24-B11-332111	2
Caelo	Mometasone furoate, micronized	16353208	7
Fagron	Mometasone furoate, micronized	16J24-B11-334371	4
Noweda	Mometasone furoate, micronized	16J24-B11-332111	1
Kehr	Mometasone furoate, micronized	16353206	1
Caelo	Mometasone furoate, micronized	16353209	12
Audor Pharma	Mometasone furoate, micronized	APMOM006/0177M	1
Caelo	Mometasone furoate, micronized	1635206	1
Euro OTC	Mometasone furoate, micronized	161000901	1
Caelo	Mometasone furoate, micronized	1610009-01	1
Caeolo/Gehe	Mometasone furoate, micronized	16J24-B11-332112	1
Fagron	Mometasone furoate, micronized	16J24-11-335793	1
Fragon/Sanacorp	Mometasone furoate, micronized	17D19-B02-339277	2
Caelo	Mometasone furoate, micronized	16J24-B11	1
Euro OTC	Mometasone furoate, micronized	16j24-B11-332111	1
Fagron	Mometasone furoate, micronized	16J24-B11-335793	3
Caelo	Mometasone furoate, micronized	16353211	3
Fagron	Mometasone furoate, micronized	17D19-B02339277	1
Caelo	Mometasone furoate, micronized	1635209	1
Caelo	Mometasone furoate, micronized	APMOM006/0117M	1
Sanacorp	Mometasone furoate, micronized	16353211	1
Caelo	Mometasone furoate, micronized	18026001	7
Caelo	Mometasone furoate, micronized	17348901	3
Euro OTC	Mometasone furoate, micronized	1711027-01	4
Caelo	Mometasone furoate, micronized	18026004	6
Caelo	Mometasone furoate, micronized	17D19-B02-34476	1
Fagron	Mometasone furoate, micronized	17D19-B02-342643	6
Fagron	Mometasone furoate, micronized	16J24-B11-332110	1
Caelo	Mometasone furoate, micronized	1711027-01	1
Fagro/Noweda	Mometasone furoate, micronized	17D19-B02-339277	1
Fragon/Sanacorp	Mometasone furoate, micronized	17D19-B02-342642	1
Sanacorp	Mometasone furoate, micronized	17D19-B02-339276	1
Fagron	Mometasone furoate, micronized	17D19B02339278	1
Caelo	Mometasone furoate, micronized	18026006	2
Fagron	Mometasone furoate, micronized	17D19-B02-347348	1

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Supplier	Substance	Batch	Spectra
Audor Pharma	Mometasone furoate, micronized	APMOM006/0517M	1
Fragon/Sanacorp	Mometasone furoate, micronized	17D19-B02-347348	1
Sanacorp	Mometasone furoate, micronized	17D19-B02-344776	1
Caelo	Mometasone furoate, micronized	17D19-B02-342643	1
Sanacorp	Mometasone furoate, micronized	MOM001/0317	1
Caelo	Mometasone furoate, micronized	MOM001/0317	1
Fagron	Mometasone furoate, micronized	17D19-B02-339277	1
Fagron	Mometasone furoate, micronized	17D19-B02-347349	1
Fagron	Mometasone furoate, micronized	18B19-B07	1
Euro OTC	Mometasone furoate, micronized	1711027	1
Fagron	Mometasone furoate, micronized	18B19-B07-341351	1
Fragon/Sanacorp	Mometasone furoate, micronized	17D19-B02-342643	2
Caelo	Mometasone furoate, micronized	17D19-B02-339277	1
Gehe 07.12.18	Mometasone furoate, micronized	171102702	1
Caelo	Mometasone furoate, micronized	18026011	1
Sanacorp	Mometasone furoate, micronized	18026001	1
Caelo	Mometasone furoate, micronized	18026007	1
Caelo/Anzag	Mometasone furoate, micronized	18026012	1
Caelo	Mometasone furoate, micronized	18026012	1
Caelo	Mometasone furoate, micronized	18B19-B07-351351	1
Audor Pharma	Mometasone furoate, micronized	APMOM301/0118M	1

- 78 332 spectra from 564 *Apo-Ident* customers from a total of 25 914 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Mometasone furoate, micronized* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mometasone furoate, micronized* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	340	0	74 156
Type B	0	445	61	126 386
Type C	0	477	120	78 332

The substance/substance group *Mometasone furoate, micronized* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9901 %)	87.9447 % (> 87.3518 %)
Type C	100.0000 % (> 99.8817 %)	79.8995 % (> 79.3970 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20850	22433	2.40	81.99
22433	22433	0.00	84.12
21602	22433	5.31	73.84
22238	22238	0.00	84.50
22887	22433	3.75	81.95
23136	23136	0.00	81.01

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Monostereates**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20691-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Monostereates; Adeps solidus (601); Glycerol monostearate 40-55%; Glycerol monostearate 60; Glycerol monostearate, emulsifying; Glyceroli monostearates 40-55%; Glyceroli monostearates 60; Glyceroli monostearates emulsificantes; Hard fat (601); Sorbitan stearate; Sorbitani stearas

Special notes

When selecting the *Monostereates* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Monostereates*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glycerol monoste...	12105705	20691	80	20120424
Caelo	Glycerol monoste...	12210401	20751	80	1407214
Caelo	Glycerol monoste...	12210401	20783	40	20120726

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sorbitan stearate	12274801	20828	40	20120924
Caelo	Glycerol monoste...	12105720	20867	40	20120424
Caelo	Hard fat (601)	13296104	20997	40	1403144
Caelo	Glycerol monoste...	13109304	21093	40	1407633
Caelo	Glycerol monoste...	13232604	21437	40	1504599
Caelo	Glycerol monoste...	14099903	21446	40	AR-15-FG-000732-02
Caelo	Glycerol monoste...	14240607	21576	40	1412120
Caelo	Glycerol monoste...	14240607	21585	40	20140815
Fagron	Sorbitan stearate	14J07-B02-299399	21885	40	AR-16-FG-004368-01
Caelo	Hard fat (601)	15184905	21974	40	20150611
Caelo	Glycerol monoste...	15286302	21982	40	20150911
Caelo	Glycerol monoste...	14308310	21993	40	20150109
Fagron	Glycerol monoste...	15E13-B03-305532	22277	40	20150703
Caelo	Glycerol monoste...	15286302	22320	40	AR-16-FG-009226-01
Caelo	Glycerol monoste...	154450	22464	40	20160225*
Caelo	Glycerol monoste...	161646	22623	40	20160727*
Caelo	Glycerol monoste...	16030301	22667	40	20160204
Caelo	Glycerol monoste...	162338	22743	40	20160822*
Caelo	Sorbitan stearate	162352	22764	40	20160826*
Caelo	Glycerol monoste...	16233804	23188	40	10052
Caelo	Hard fat (601)	172178	23690	40	20170817*
Caelo	Sorbitan stearate	17030805	23706	40	20170210
Caelo	Sorbitan stearate	172564	23831	40	20171027*
Caelo	Glycerol monoste...	180683	24025	40	20180430*
Caelo	Glycerol monoste...	182462	24371	40	20181008*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1200 spectra of 28 reference samples from the substance/substance group *Monostereates*. These samples are listed above in the [calibration samples](#) section.
- 73 296 spectra from a total of 1598 batches from further 368 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.

- 1160 spectra of 31 reference samples from the substance/substance group *Monostereates*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glycerol monostearate, emuls. ...	11079309	20621	40
Caelo	Glycerol monostearate 60	11272902	20677	80
Fagron	Sorbitan stearate	11I26-N09	20736	40
Fagron	Glycerol monostearate, emuls. ...	11I15-N09	20746	80
Fagron	Glycerol monostearate, emuls. ...	12B14-N10	20786	40
Caelo	Glycerol monostearate 60	13232604	21437 [†]	20
Caelo	Glycerol monostearate 40-55%	14099903	21446 [†]	20
Caelo	Hard fat (601)	14099604	21488	40
Fagron	Glycerol monostearate 40-55%	14C12-B40-292622	21545	60
Caelo	Glycerol monostearate, emuls. ...	14240607	21576 [†]	20
Caelo	Glycerol monostearate, emuls. ...	14240607	21585 [†]	20
Fagron	Sorbitan stearate	14J07-B02-299399	21885 [†]	20
Caelo	Hard fat (601)	15184905	21974 [†]	20
Caelo	Glycerol monostearate 60	15286302	21982 [†]	20
Caelo	Glycerol monostearate, emuls. ...	14308310	21993 [†]	20
Fagron	Glycerol monostearate 40-55%	15E13-B03-305532	22277 [†]	20
Caelo	Glycerol monostearate, emuls. ...	14308310	22278	60
Caelo	Glycerol monostearate 60	15286302	22320 [†]	20
Caelo	Glycerol monostearate, emuls. ...	14308310	22341	60
Caelo	Glycerol monostearate 40-55%	154450	22464 [†]	20
Caelo	Glycerol monostearate 60	162338	22646	40
Caelo	Hard fat (601)	162364	22648	40
Caelo	Glycerol monostearate 60	162338	22741	40
Caelo	Glycerol monostearate 60	162338	22742	40
Caelo	Glycerol monostearate 60	162338	22744	40
Caelo	Hard fat (601)	162364	22766	40
Caelo	Sorbitan stearate	171781	23622	40
Caelo	Glycerol monostearate, emuls. ...	172585	23822	40
Caelo	Sorbitan stearate	180432	24021	40
Caelo	Glycerol monostearate 40-55%	180447	24267	40
Caelo	Sorbitan stearate	183125	24377	40

- 125 732 spectra from a total of 2766 batches from further 777 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.

- 194 spectra from 98 *Apo-Ident* customers from 85 batches from the substance/substance group *Monostereates*.

Supplier	Substance	Batch	Spectra
Spangropharm	Glycerol monostearate 40-55%	80402468	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	Glycerol monostearate 40-55%	12A27-N11	1
Caelo	Glycerol monostearate 40-55%	12105729	1
Fagron	Glycerol monostearate 40-55%	12K05-N06	1
Caelo	Glycerol monostearate 40-55%	13156601	2
Caelo	Glycerol monostearate 40-55%	12105704	1
Fagron	Glycerol monostearate 40-55%	7G19-N09	1
Caelo	Glycerol monostearate 40-55%	13221303	2
Caelo	Glycerol monostearate 40-55%	131156602	1
Caelo	Glycerol monostearate 40-55%	13221308	1
Caesar/Noweda	Glycerol monostearate 40-55%	13221311	2
Caelo	Glycerol monostearate 40-55%	14169710	1
Fagron	Glycerol monostearate 40-55%	15280903	1
Caelo	Glycerol monostearate 40-55%	15280903	2
Caelo	Glycerol monostearate 40-55%	15280904	2
Caelo	Glycerol monostearate 40-55%	15445007	5
Caelo	Glycerol monostearate 40-55%	14359407	1
Caelo	Glycerol monostearate 40-55%	15445010	1
Caelo	Glycerol monostearate 40-55%	18044702	1
Caelo	Glycerol monostearate 40-55%	15445011	1
Caelo	Glycerol monostearate 40-55%	15445014	1
Caelo	Glycerol monostearate 40-55%	18044701	2
Anzag	Glycerol monostearate 60	12180502	1
Caelo	Glycerol monostearate 60	13018201	3
Caelo	Glycerol monostearate 60	1301821	1
Caelo	Glycerol monostearate 60	12001001	1
Caelo	Glycerol monostearate 60	13109304	9
Caesar/Noweda	Glycerol monostearate 60	13109304	1
Phonix	Glycerol monostearate 60	13109304	1
Caesar u Loretz	Glycerol monostearate 60	13109304	1
Audor Pharma	Glycerol monostearate 60	13232604	1
Caelo	Glycerol monostearate 60	13232604	3
Caelo	Glycerol monostearate 60	14012002	4
Caesar u Loretz	Glycerol monostearate 60	14012002	1
Caelo	Glycerol monostearate 60	15009203	13
Fagron	Glycerol monostearate 60	15009203	1
Noweda	Glycerol monostearate 60	15009203	1
Caelo	Glycerol monostearate 60	15286302	3
Caesar & Loretz/Noweda	Glycerol monostearate 60	15009203	1
Caelo	Glycerol monostearate 60	15286308	3
Caelo	Glycerol monostearate 60	15286307	2
Caelo	Glycerol monostearate 60	16233804	3
Euro OTC	Glycerol monostearate 60	16233804	1
Caelo	Glycerol monostearate 60	17061703	3
Caelo	Glycerol monostearate 60	17167803	2
Caelo	Glycerol monostearate 60	17167804	3
Caelo	Glycerol monostearate 60	18068303	2
Fagron	Sorbitan stearate	12E30-N14	1
Fagron	Sorbitan stearate	5052	1
Caelo	Sorbitan stearate	13B19-N01	1
Fagron	Sorbitan stearate	13B19-N01	1
Fagron	Sorbitan stearate	13D10N10	1
Caelo	Sorbitan stearate	12274813	2
Fagron	Sorbitan stearate	13D10-N10	1
Caelo	Sorbitan stearate	12274807	1
Caelo	Sorbitan stearate	13209410	1
Caelo	Sorbitan stearate	13209418	2
Phonix	Sorbitan stearate	13209418	1
anzag	Sorbitan stearate	14195	1
Caelo	Sorbitan stearate	14038504	1
Caelo	Sorbitan stearate	13209409	2

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Supplier	Substance	Batch	Spectra
Caelo	Sorbitan stearate	13209419	3
Cealo	Sorbitan stearate	13209409	1
Caelo	Sorbitan stearate	14038510	1
Caelo	Sorbitan stearate	13209417	3
Caelo	Sorbitan stearate	14038511	2
Caelo	Sorbitan stearate	14218803	3
Caelo	Sorbitan stearate	14218808	3
Fagron	Sorbitan stearate	14J07-B02-299399	1
Ichthylol/Phoenix	Sorbitan stearate	14372803	1
Caelo	Sorbitan stearate	26031507	1
Nachprüfung	Sorbitan stearate		1
Caelo	Sorbitan stearate	14218804	1
Caelo	Sorbitan stearate	14372803	1
Caelo	Sorbitan stearate	15300302	7
Caelo	Sorbitan stearate	15300308	4
Caelo	Sorbitan stearate	15415202	7
Caelo	Sorbitan stearate	16235207	8
ALH	Sorbitan stearate	16235202	1
Caelo	Sorbitan stearate	17030805	2
Caelo	Sorbitan stearate	17178102	5
Caelo	Sorbitan stearate	17345402	1
Caelo	Hard fat (601)	13296104	1
Caelo	Hard fat (601)	15184901	1
Caelo	Hard fat (601)	14099608	1
Noweda	Glycerol monostearate, emuls...	11079301	1
Caelo	Glycerol monostearate, emuls...	11079308	1
Caelo	Glycerol monostearate, emuls...	13109405	2
Caelo	Glycerol monostearate, emuls...	13109410	1
Caelo	Glycerol monostearate, emuls...	1420607	1
Caelo	Glycerol monostearate, emuls...	13109402	1
Gehe	Glycerol monostearate, emuls...	14240605	2
Caelo	Glycerol monostearate, emuls...	14240607	1
Caelo	Glycerol monostearate, emuls...	14240611	1
Caelo	Glycerol monostearate, emuls...	14308310	3
Caelo	Glycerol monostearate, emuls...	16030301	2
Caelo	Glycerol monostearate, emuls...	16030304	2
Caelo	Glycerol monostearate, emuls...	16164604	1
Caelo	Glycerol monostearate, emuls...	16164606	1

- 78 735 spectra from 565 *Apo-Ident* customers from a total of 26 054 batches from a further 689 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Monostereates* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Monostereates* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	1200	0	73 296
Type B	0	1024	136	125 732
Type C	0	188	6	78 735

The substance/substance group *Monostereates* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 99.5000 %)
Type B	100.0000 % (> 99.9901 %)	88.2759 % (> 88.0172 %)
Type C	100.0000 % (> 99.8817 %)	96.9072 % (> 95.3608 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20997	20997	0.00	44.25
21576	21576	0.00	35.33
21585	21576	1.66	35.13
21974	20997	7.63	44.50
21982	22320	3.13	37.39
22320	22320	0.00	38.71
24371	24371	0.00	41.03
20691	21446	7.89	39.17
20867	21446	21.08	38.88
21446	21446	0.00	39.55
21093	21093	0.00	42.61
22743	22743	0.00	41.13
22277	21446	22.65	35.83
22623	22623	0.00	38.97
21437	21437	0.00	32.26
23188	23188	0.00	34.60
20751	20751	0.00	32.53
20783	20751	2.98	32.45
21993	20751	10.81	31.85
22667	20751	8.89	31.49
23690	23690	0.00	45.85
20828	22764	18.97	53.62
22764	22764	0.00	51.43
23706	22764	3.33	51.73
23831	23831	0.00	48.05

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24025	24025	0.00	45.99
21885	21885	0.00	49.44
22464	22464	0.00	43.98

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Mupirocin calcium
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20781-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mupirocin calcium; Mupirocinum calcii

Special notes

When selecting the *Mupirocin calcium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Mupirocin calcium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Mupirocin calcium	12E02-N07	20781	40	1401556
Caelo	Mupirocin calcium	14276602	21745	40	20141103
Caelo	Mupirocin calcium	161184	22454	40	20160504*

Validation samples

A total of 280 317 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 *Mupirocin calcium*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Mupirocin calcium*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mupirocin calcium	14276602	21745 [†]	20
Caelo	Mupirocin calcium	161184	22454 [†]	20
Fagron	Mupirocin calcium	15H13-B01-316111	23213	40
Caelo	Mupirocin calcium	161608	23860	40

- 126 772 spectra from a total of 2785 batches from further 781 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 5 *Apo-Ident* customers from 8 batches from the substance/substance group *Mupirocin calcium*.

*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	Mupirocin calcium	83200301013	1
Fagron	Mupirocin calcium	14B03-B30-297291	1
Caelo	Mupirocin calcium	17356502	1
Fagron	Mupirocin calcium	15H13-B01	1
Caelo	Mupirocin calcium	9041801	1
Fagron	Mupirocin calcium	17F21-B03-339080	1
Fagron	Mupirocin calcium	83200340116	1
Caelo	Mupirocin calcium	24041801	1

- 78 921 spectra from 565 *Apo-Ident* customers from a total of 26 129 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Mupirocin calcium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mupirocin calcium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	115	5	126 772
Type C	0	7	1	78 921

The substance/substance group *Mupirocin calcium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	95.8333 % (> 93.3333 %)
Type C	100.0000 % (> 99.8818 %)	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
20781	20781	0.00	52.63
21745	22454	5.73	52.13
22454	22454	0.00	51.43

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Naloxone hydrochloride dihydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20957-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Naloxone hydrochloride dihydrate; Naloxoni hydrochloridum dihydricum

Special notes

When selecting the *Naloxone hydrochloride dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Naloxone hydrochloride dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Naloxone hydroch...	13D22-N07	20957	40	1402059
Fagron	Naloxone hydroch...	13L12-B03	21271	40	20140113
Audor	Naloxone hydroch...	AP13501078IIN	22811	40	20160429
Caelo	Naloxone hydroch...	163577	23039	40	20170306*

Validation samples

A total of 280317 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 *Naloxone hydrochloride dihydrate*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 *Naloxone hydrochloride dihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Naloxone hydrochloride dihyd...	15322517	22828	40
Caelo	Naloxone hydrochloride dihyd...	170441	23862	40

- 126812 spectra from a total of 2787 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 5 *Apo-Ident* customers from 12 batches from the substance/substance group *Naloxone hydrochloride dihydrate*.

*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
Fagron	Naloxone hydrochloride dihyd...	11/23-N01	1
Fagron	Naloxone hydrochloride dihyd...	12G19-N02	2
Fagron	Naloxone hydrochloride dihyd...	12-00071	2
Fagron	Naloxone hydrochloride dihyd...	12G19-N02	1
Fagron	Naloxone hydrochloride dihyd...	13L12-B03-289511	1
Fagron	Naloxone hydrochloride dihyd...	15E28-B01-308324	3
Fagron	Naloxone hydrochloride dihyd...	14F20-B02-296077	1
Fagron	Naloxone hydrochloride dihyd...	15H04-B09-314068	1
Fagron	Naloxone hydrochloride dihyd...	15B06-B02-304421	1
Fagron	Naloxone hydrochloride dihyd...	15H04-B09	3
Audor Pharma	Naloxone hydrochloride dihyd...	AP13501078N	1
Fagron	Naloxone hydrochloride dihyd...	15K11-B05-319571	1

- 78 911 spectra from 565 *Apo-Ident* customers from a total of 26 125 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Naloxone hydrochloride dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naloxone hydrochloride dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	80	0	126 812
Type C	0	11	7	78 911

The substance/substance group *Naloxone hydrochloride dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8817 %)	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
23039	23039	0.00	49.89
20957	20957	0.00	46.78
21271	20957	5.73	44.97
22811	20957	12.24	48.67

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Naphazoline hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20899-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Naphazoline hydrochloride; Naphazolini hydrochloridum

Special notes

When selecting the *Naphazoline hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Naphazoline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Naphazoline hydr...	12375211	20899	40	20130108
Euro OTC	Naphazoline hydr...	1407034-01	21623	40	AR-15-FG-007847-01
Euro OTC	Naphazoline hydr...	1506015	21859	40	20150727*

Validation samples

A total of 280317 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 *Naphazoline hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 6 reference samples from the substance/substance group *Naphazoline hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Naphazoline hydrochloride	12375211	21397	60
Caelo	Naphazoline hydrochloride	12375211	21398	60
Euro OTC	Naphazoline hydrochloride	1407034-01	21623 [†]	20
Euro OTC	Naphazoline hydrochloride	1506015	21859 [†]	20
Euro OTC	Naphazoline hydrochloride	1607041	22753	40
Euro OTC	Naphazoline hydrochloride	1704005	23385	40

- 126652 spectra from a total of 2784 batches from further 781 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.

- 133 spectra from 99 *Apo-Ident* customers from 70 batches from the substance/substance group *Naphazoline hydrochloride*.

*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
Fagron	Naphazoline hydrochloride	11J13-N08	1
Fagron	Naphazoline hydrochloride	11/05-N02	1
Euro OTC	Naphazoline hydrochloride	113031-01	1
Fagron	Naphazoline hydrochloride	4309I-01885	1
Caelo	Naphazoline hydrochloride	1206037	1
Caelo	Naphazoline hydrochloride	2275310	1
Caelo	Naphazoline hydrochloride	11081107	2
Caelo	Naphazoline hydrochloride	9285103	2
Euro OTC	Naphazoline hydrochloride	1103031-02	1
Phönix	Naphazoline hydrochloride	586550002	1
Euro OTC	Naphazoline hydrochloride	1206037-01	1
Fagron	Naphazoline hydrochloride	11K25-N03	2
Fagron	Naphazoline hydrochloride	13C11-N07	4
Fagron	Naphazoline hydrochloride	12K29-N01o256/310	1
Fagron	Naphazoline hydrochloride	11I05-N02	2
Euro OTC	Naphazoline hydrochloride	1206037-02	4
Fagron	Naphazoline hydrochloride	4509E-01885	2
Fagron	Naphazoline hydrochloride	13A07-N06	4
Eurho/Phoenix	Naphazoline hydrochloride	4413I-01885	1
Fagron	Naphazoline hydrochloride	13C11N07	1
Fagron	Naphazoline hydrochloride	13K27-N04	12
Caelo	Naphazoline hydrochloride	12375211	1
Fagron	Naphazoline hydrochloride	60494000113K27-N04	1
Caelo	Naphazoline hydrochloride	1216203	1
Caleo /Herba	Naphazoline hydrochloride	9285103	1
Caelo	Naphazoline hydrochloride	15071404	1
Caelo	Naphazoline hydrochloride	1307020-02	1
Fagron	Naphazoline hydrochloride	13k27-n04	1
Euro OTC	Naphazoline hydrochloride	14070034-01	1
Euro OTC	Naphazoline hydrochloride	1307020-03	2
Fagron	Naphazoline hydrochloride	13103-B03-295105	2
Fagron	Naphazoline hydrochloride	1303-B03	1
Fagron	Naphazoline hydrochloride	13I03-B03-295105	2
Fagron	Naphazoline hydrochloride	13I03-B03-305291	2
Fagron	Naphazoline hydrochloride	13/03-B03-295105	2
Fargon	Naphazoline hydrochloride	13/03-B03-295105	1
Euro OTC	Naphazoline hydrochloride	1407034-02	4
Noweda-Fragon	Naphazoline hydrochloride	1303B03305291	1
Caelo	Naphazoline hydrochloride	15223301	2
Fagron	Naphazoline hydrochloride	13I03-B03	1
Fagron	Naphazoline hydrochloride	13/03-B03	1
Euro OTC	Naphazoline hydrochloride	1506015-01	2
Fagron	Naphazoline hydrochloride	13/03-B03-305291	1
EuRho	Naphazoline hydrochloride	1114I-001885	1
Euro OTC	Naphazoline hydrochloride	1506015-02	7
Caelo	Naphazoline hydrochloride	1506015-2	1
Euro OTC	Naphazoline hydrochloride	150601502	1
Caelo	Naphazoline hydrochloride	12176203	2
Euro OTC	Naphazoline hydrochloride	1407034-01	1
Fagron	Naphazoline hydrochloride	15J05-B05	2
Caelo	Naphazoline hydrochloride	15223303	1
Euro OTC	Naphazoline hydrochloride	1607041-01	3
Caelo	Naphazoline hydrochloride	16174101	3
Fagron	Naphazoline hydrochloride	15J05-B05-322527	1
Fagron	Naphazoline hydrochloride	13103-803-305291	1
Fagron	Naphazoline hydrochloride	13/03-B03305291	1
Euro OTC	Naphazoline hydrochloride	1607041	1
Caelo	Naphazoline hydrochloride	140703402	1
Fagron	Naphazoline hydrochloride	15J05-B05-326850	3
Euro OTC	Naphazoline hydrochloride	1407034-03	1

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Supplier	Substance	Batch	Spectra
Gehe/EuRo	Naphazoline hydrochloride	1607041-01	1
Fagron	Naphazoline hydrochloride	15J05B05326850	1
Fagron	Naphazoline hydrochloride	17C02-B05-332933	4
Fagron	Naphazoline hydrochloride	17C02-B05	1
Caelo	Naphazoline hydrochloride	15J05-B05/171025NHC	1
Fargon/Apo.am Park	Naphazoline hydrochloride	539580002	1
Fagron	Naphazoline hydrochloride	15J05-B05-330834	3
Fagron	Naphazoline hydrochloride	17C02-B05-335313	5
Fagron	Naphazoline hydrochloride	17c02-b05-335313	1
Fagron	Naphazoline hydrochloride	17C02-B05-335113	1
Fagron	Naphazoline hydrochloride	17C02-B05-343566	3
Fargon/Noweda	Naphazoline hydrochloride	17C02-B05-346657	1
Caelo	Naphazoline hydrochloride	18119302	1

- 78 796 spectra from 565 *Apo-Ident* customers from a total of 26 067 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Naphazoline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naphazoline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	240	0	126 652
Type C	0	127	6	78 796

The substance/substance group *Naphazoline hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.8817 %)	95.4887 % (> 93.2331 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21859	21859	0.00	40.79
20899	21623	8.92	47.42
21623	21623	0.00	41.10

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Naphazoline nitrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20501-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Naphazoline nitrate; Naphazolini nitras

Special notes

When selecting the *Naphazoline nitrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Naphazoline nitrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Naphazoline nitr...	12L10-N03	20846	40	20121217
Fagron	Naphazoline nitr...	12J08-B40-287904	21808	40	20131129
Euro OTC	Naphazoline nitr...	1512033	22302	40	20160126*

Validation samples

A total of 280317 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 *Naphazoline nitrate*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 *Naphazoline nitrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Naphazoline nitrate	12J08-B40-287904	21808 [†]	20
Euro OTC	Naphazoline nitrate	1512033	22302 [†]	20
Fagron	Naphazoline nitrate	16A14-B03-327343	23164	40
Euro OTC	Naphazoline nitrate	1512033-01	23275	40
Euro OTC	Naphazoline nitrate	1810016	24341	40

- 126732 spectra from a total of 2784 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 11 spectra from 11 *Apo-Ident* customers from 11 batches from the substance/substance group *Naphazoline nitrate*.

*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
Fagron	Naphazoline nitrate	21021304	1
Audor Pharma	Naphazoline nitrate	12I21-N05	1
Fagron	Naphazoline nitrate	12J08B40-294166	1
Fagron	Naphazoline nitrate	11I05-N03	1
Fagron	Naphazoline nitrate	12/21-N05	1
Fagron	Naphazoline nitrate	12J08-B40-294166	1
Fagron	Naphazoline nitrate	12J08-B40	1
Fagron	Naphazoline nitrate	12j08-b40-303401	1
Fagron	Naphazoline nitrate	140214N	1
Fagron	Naphazoline nitrate	16A14-B03-322534	1
Fagron	Naphazoline nitrate	16A14-B03-327343	1

- 78 918 spectra from 565 *Apo-Ident* customers from a total of 26 126 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Naphazoline nitrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naphazoline nitrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	0	126 732
Type C	0	10	1	78 918

The substance/substance group *Naphazoline nitrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8818 %)	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
22302	22302	0.00	34.06
20846	22302	6.20	34.19
21808	22302	1.89	34.56

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Naproxen**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22316-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Naproxen; Naproxenum

Special notes

When selecting the *Naproxen* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Naproxen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Naproxen	15F18-B03-309492	22316	30	AR-16-FG-008486-02
Fagron	Naproxen	15F18-B03-315691	22327	30	20150703
Fagron	Naproxen	16B04-B09-326261	23105	40	20160229

Validation samples

A total of 280 317 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 *Naproxen*. These samples are listed above in the [calibration samples](#) section.
- 74 396 spectra from a total of 1620 batches from further 372 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 [†].

- 70 spectra of 3 reference samples from the substance/substance group *Naproxen*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Naproxen	15F18-B03-309492	22316 [†]	15
Fagron	Naproxen	15F18-B03-315691	22327 [†]	15
Fagron	Naproxen	17C10-B03-336472	23763	40

- 126 822 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 26 spectra from 5 *Apo-Ident* customers from 2 batches from the substance/substance group *Naproxen*.

Supplier	Substance	Batch	Spectra
Fagron	Naproxen	16B04-B09-321569	24
Fagron	Naproxen	13E31-B40-287536	2

[†]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*.

- 78 903 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Naproxen* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naproxen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 396
Type B	0	70	0	126 822
Type C	0	25	1	78 903

The substance/substance group *Naproxen* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 91.4286 %)
Type C	100.0000 % (> 99.8817 %)	96.1538 % (> 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
22316	22316	0.00	46.74
22327	22316	0.90	46.88
23105	22316	3.90	43.74

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Neomycin sulfate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20544-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Neomycin sulfate; Neomycin sulphate; Neomycini sulfas

Special notes

When selecting the *Neomycin sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Neomycin sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Neomycin sulfate	1303033-03	21771	40	AR-15-FG-016582-01
Caelo	Neomycin sulfate	13062923	21814	40	AR-15-FG-016581-01
Fagron	Neomycin sulfate	14C27-B05-302516	21894	40	1604527
Fagron	Neomycin sulfate	14C27-B05-302517	21961	40	20140418
Caelo	Neomycin sulfate	13062923	22276	30	20130315
Euro OTC	Neomycin sulfate	1601046	22381	30	20160212*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 6 reference samples from the substance/substance group *Neomycin sulfate*. These samples are listed above in the [calibration samples](#) section.
- 74 276 spectra from a total of 1618 batches from further 372 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 [†].

- 425 spectra of 13 reference samples from the substance/substance group *Neomycin sulfate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Neomycin sulfate	1102043-02	20758	40
Euro OTC	Neomycin sulfate	1303033-03	21771 [†]	20
Caelo	Neomycin sulfate	13062923	21814 [†]	20
Fagron	Neomycin sulfate	14C27-B05-302516	21894 [†]	20
Fagron	Neomycin sulfate	14C27-B05-302517	21961 [†]	20
Caelo	Neomycin sulfate	13062923	22276 [†]	15
Euro OTC	Neomycin sulfate	1601046	22381 [†]	15
Caelo	Neomycin sulfate	15237602	22389	40
Caelo	Neomycin sulfate	161650	23856	30
Euro OTC	Neomycin sulfate	1802005	23952	40
Fagron	Neomycin sulfate	14C27-B05-302516	21894SI	60
Fagron	Neomycin sulfate	14C27-B05-302517	21961SI	60
Caelo	Neomycin sulfate	13062923	22276SI	45

- 126 467 spectra from a total of 2780 batches from further 781 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.

- 347 spectra from 187 *Apo-Ident* customers from 106 batches from the substance/substance group *Neomycin sulfate*.

Supplier	Substance	Batch	Spectra
Fagron	Neomycin sulfate	11C21-N10	2
Caelo	Neomycin sulfate	9105316	1
Caesar & Loretz GmbH, 4...	Neomycin sulfate	11/19-N14	1
Fagron	Neomycin sulfate	11/19-N14	4
Fagron	Neomycin sulfate	12I19-N14	1
Caelo	Neomycin sulfate	10157505	5
Caesar&lorenz,Phoenix	Neomycin sulfate	12C13-N04	1
Euro OTC	Neomycin sulfate	1102043	2
Euro OTC	Neomycin sulfate	1102043-02	7
Caelo	Neomycin sulfate	24111203	1
Gehe	Neomycin sulfate	183360-0009	1
Caelo	Neomycin sulfate	1102043-02	1
Euro OTC	Neomycin sulfate	1102043-01	3
Fagron	Neomycin sulfate	12C13-N04	4
Fagron	Neomycin sulfate	12H23-N04	6
Caelo	Neomycin sulfate	12175401	4
Pfizer/Euro OCT Pharma	Neomycin sulfate	1102043-02	2
Alliance Healthcare	Neomycin sulfate	1102043-03	1
Euro OTC	Neomycin sulfate	1102043-03	4
Caelo	Neomycin sulfate	11C21-N10	1
AHD	Neomycin sulfate	11/19-N14	1
Euro OTC	Neomycin sulfate	1303033-01	10
Fagron	Neomycin sulfate	13D10-N05	1
Fagron	Neomycin sulfate	13D10-N05	5
Caelo	Neomycin sulfate	12276405	1
aurica/phoenix	Neomycin sulfate	1102043-02	1
EuRho	Neomycin sulfate	1102043-02	1
Phönix	Neomycin sulfate	13D10-N05	1
Caelo	Neomycin sulfate	13G09-N07	1
Fagron	Neomycin sulfate	13G09-N07	12
Alliance Health 13.01.204	Neomycin sulfate	1303033-01	2
Caelo	Neomycin sulfate	5/AKD35	1
Fagron	Neomycin sulfate	10121-N01	1
EuRho/Sanacorp	Neomycin sulfate	1102043-03	1
Fagron	Neomycin sulfate	13G09N07	2
Fagron	Neomycin sulfate	13G09-N06	1
phnoix	Neomycin sulfate	130303301	1
siehe WE-Prüfprotokoll	Neomycin sulfate	19/12	1
Noweda	Neomycin sulfate	1102043-02	1
Fagron	Neomycin sulfate	13G09-N070129/340	1
Caelo	Neomycin sulfate	12276410	2
Caelo	Neomycin sulfate	9051402	1
Ashland/Sanacorp	Neomycin sulfate	1303033-02	1
Land/Phönix	Neomycin sulfate	13062905	2
Euro OTC	Neomycin sulfate	1303033-02	14
	Neomycin sulfate	13G09-N07	2
VDL;24.6.14; 3,55EUR	Neomycin sulfate	1303033-02	2
Caelo	Neomycin sulfate	563313062905	1

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Supplier	Substance	Batch	Spectra
Pfizer USA / Phönix	Neomycin sulfate	1303033-02	1
Fagron	Neomycin sulfate	13K15-B33-288073	1
Fagron	Neomycin sulfate	13K15-B33-288069	2
Caelo	Neomycin sulfate	13062905	2
Euro OTC	Neomycin sulfate	1303033-03	15
Fagron	Neomycin sulfate	14A31-B02-294696	3
Fagron	Neomycin sulfate	F08469	1
AHD	Neomycin sulfate	14A31-B02-294698	2
Caelo	Neomycin sulfate	13D10N05	1
Fagron	Neomycin sulfate	F08469	1
phoenix 13.11.14	Neomycin sulfate	1303033-03	1
Fagron	Neomycin sulfate	4312I-01926	1
fargron	Neomycin sulfate	14A31-B02-294698	1
Gehe	Neomycin sulfate	194A-01926	1
Caelo	Neomycin sulfate	1303033-03	1
Caelo	Neomycin sulfate	5/AKD36	1
	Neomycin sulfate	1303033-03	1
Fagron	Neomycin sulfate	14A31B02294696	1
Caelo	Neomycin sulfate	14A31-B02-294696	1
Fagron	Neomycin sulfate	14A31-B02-294698	1
Fagron	Neomycin sulfate	14A31-B02-294697	1
Caelo	Neomycin sulfate	13062908	1
Fagron	Neomycin sulfate	14A31B02	2
Caelo	Neomycin sulfate	13062923	4
Euro OTC	Neomycin sulfate	1303001-03	1
Fagron	Neomycin sulfate	14A31-B02	2
Taoasis/Phoenix	Neomycin sulfate	1502004-01	1
Fagron	Neomycin sulfate	14A31-B02-296724	1
Euro OTC	Neomycin sulfate	1502004-01	14
Caelo	Neomycin sulfate	13062922	1
HenryLamotte	Neomycin sulfate	1502004-01	3
Fagron	Neomycin sulfate	14A31-B02-302519	4
Euro/Phönix	Neomycin sulfate	1502004-01	1
Fagron	Neomycin sulfate	14c27-B05-302516	1
Fagron	Neomycin sulfate	14C27-B05	1
Euro OTC	Neomycin sulfate	1502004	1
Euro OTC	Neomycin sulfate	G73890	1
Euro OTC	Neomycin sulfate	L34419	3
Fagron	Neomycin sulfate	14C27-B05-302516	2
Fagron	Neomycin sulfate	14C27-B05-302517	1
Fagron	Neomycin sulfate	1502004-01	2
Fagron	Neomycin sulfate	15J09-B04-314017	4
Caesar&Loretz/Noweda	Neomycin sulfate	15298904	1
EuRho/Sanacorp	Neomycin sulfate	1502004-01	2
Caelo	Neomycin sulfate	15237602	4
Caelo	Neomycin sulfate	15298902	1
caesar&loretz,AHC,7.3.16	Neomycin sulfate	13062923	1
Euro OTC	Neomycin sulfate	16019046-01	1
Fagron	Neomycin sulfate	15J09-B04-314015	4
Noweda	Neomycin sulfate	15298902	1
Fagron	Neomycin sulfate	15J27-B07	1
Sanacorp	Neomycin sulfate	15298902	1
Cealo/AHD	Neomycin sulfate	15J09-B04-314017	1
Euro OTC	Neomycin sulfate	1601046-01	18
Jenne	Neomycin sulfate	15237602	1
Caelo	Neomycin sulfate	130303303	2
Euro OTC	Neomycin sulfate	160104601	1
Caelo	Neomycin sulfate	16122601	1
Euro OTC	Neomycin sulfate	1502004-02	3
Fagron	Neomycin sulfate	15J09-B04314015	1

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Supplier	Substance	Batch	Spectra
Caesar&Loretz,AHC,05.09...	Neomycin sulfate	15237602	1
Fagron	Neomycin sulfate	15i09-B04-314015	1
Caelo	Neomycin sulfate	13062921	1
Fagron	Neomycin sulfate	15J09-B04	1
Euro OTC	Neomycin sulfate	151116N	1
Caelo	Neomycin sulfate	16122611	2
apo-ident.;4,45EUR; Sanac...	Neomycin sulfate	1601046-01	1
Fragon/Phoenix	Neomycin sulfate	15J09-B04322943	1
Caelo	Neomycin sulfate	1601046-01	2
euro	Neomycin sulfate	1502004-02	2
Caelo	Neomycin sulfate	16122612	3
Caelo	Neomycin sulfate	16122618	1
Euro OTC	Neomycin sulfate	1502004-03	10
Fagron	Neomycin sulfate	16A20-B10-327433	2
Fagron	Neomycin sulfate	16A20-B01-327433	1
Fagron	Neomycin sulfate	M71862	2
Caesar&Loretz GmbH,18.0...	Neomycin sulfate	16122612	1
Caelo	Neomycin sulfate	16165004	1
Caelo	Neomycin sulfate	1502004-03	1
Fagron	Neomycin sulfate	1502004-03	1
Fagron	Neomycin sulfate	16A20-B10	1
GEHE	Neomycin sulfate	1502001-03	1
Caelo	Neomycin sulfate	16B10-B50-328165	1
Fagron	Neomycin sulfate	16B10-B50-328165	4
Fagron	Neomycin sulfate	17B14-B08	1
Caelo	Neomycin sulfate	161650145351	1
Euro OTC	Neomycin sulfate	1601046-02	11
Caelo	Neomycin sulfate	16165008	1
euro//Noweda	Neomycin sulfate	1601046-02	1
Fagron	Neomycin sulfate	17B14-B08-334000	1
cealo	Neomycin sulfate	1502004-03	1
Fagron	Neomycin sulfate	17G05-B04	1
Caelo	Neomycin sulfate	16165016	5
Noweda/Euro	Neomycin sulfate		1
Caelo	Neomycin sulfate	16165018	3
Caelo	Neomycin sulfate	1601046	1
Caelo	Neomycin sulfate	1601046-02	1
Eurho	Neomycin sulfate	1601046-02	1
Kehr	Neomycin sulfate	1601046-02	1
Fagron	Neomycin sulfate	17F12-B04	1
Pharmacia & Upjohn Comp...	Neomycin sulfate	16122623	1
Fagron	Neomycin sulfate	100810-112-91	1
Caelo	Neomycin sulfate	N05780	1
Pharmacia & Upjohn Comp...	Neomycin sulfate	16165017	1
Euro OTC	Neomycin sulfate	1802005-01	6
Euro OTC	Neomycin sulfate	1601046-1	1
Caelo	Neomycin sulfate	1802005-01	1
Gehe 23.11.18	Neomycin sulfate	1802005-01	1

- 78 582 spectra from 565 *Apo-Ident* customers from a total of 26 034 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Neomycin sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Neomycin sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	220	0	74 276
Type B	0	362	63	126 467
Type C	0	306	41	78 582

The substance/substance group *Neomycin sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9901 %)	85.1765 % (> 84.4706 %)
Type C	100.0000 % (> 99.8817 %)	88.1844 % (> 87.3199 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21961	21814	6.59	24.53
22276	21814	3.23	21.78
22381	22381	0.00	26.71
21771	21771	0.00	21.89
21814	21814	0.00	21.38
21894	21894	0.00	42.93

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Neostigmine bromide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20717-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Neostigmine bromide; Neostigmini bromidum

Special notes

When selecting the *Neostigmine bromide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Neostigmine bromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Neostigmine brom...	10144105	20717	40	20100616
Caelo	Neostigmine brom...	12172304	20990	40	1403163
Caelo	Neostigmine brom...	14256802	21816	40	AR-15-FG-014460-01
Caelo	Neostigmine brom...	15228101	21919	40	20151002
Caelo	Neostigmine brom...	14256802	21816SI	40	AR-15-FG-014460-01
Caelo	Neostigmine brom...	15228101	21919SI	40	20151002

Validation samples

A total of 280 317 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 *Neostigmine bromide*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1619 batches from further 372 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 8 reference samples from the substance/substance group *Neostigmine bromide*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Neostigmine bromide	14256802	21816 [†]	20
Caelo	Neostigmine bromide	15228101	21919 [†]	20
Caelo	Neostigmine bromide	171319	23369	40
Caelo	Neostigmine bromide	17131901	23373	40
Caelo	Neostigmine bromide	14256802	21816SI [†]	20
Caelo	Neostigmine bromide	15228101	21919SI [†]	20
Caelo	Neostigmine bromide	171319	23369SI	40
Caelo	Neostigmine bromide	17131901	23373SI	40

- 126 652 spectra from a total of 2785 batches from further 781 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*.

- 23 spectra from 8 *Apo-Ident* customers from 13 batches from the substance/substance group *Neostigmine bromide*.

Supplier	Substance	Batch	Spectra
Caelo	Neostigmine bromide	12172301	1
Caelo	Neostigmine bromide	12172304	1
Gehe	Neostigmine bromide	12172307	1
Gehe	Neostigmine bromide	12172301	1
Caelo	Neostigmine bromide	13177201	1
Gehe	Neostigmine bromide	13177201	1
Caelo	Neostigmine bromide	131772303A	1
Caelo	Neostigmine bromide	131772303B	1
Caelo	Neostigmine bromide	13177203	2
Caelo	Neostigmine bromide	13177206	5
Caelo	Neostigmine bromide	14256802	3
Caelo	Neostigmine bromide	15228101	1
Caelo	Neostigmine bromide	15228103	1
Hetterich/Noewda	Neostigmine bromide	17131901	1
Sanacorp	Neostigmine bromide	18024902	1
Caelo	Neostigmine bromide	17131901	1

- 78 906 spectra from 565 *Apo-Ident* customers from a total of 26 124 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Neostigmine bromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Neostigmine bromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	240	0	126 652
Type C	0	23	0	78 906

The substance/substance group *Neostigmine bromide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 73.9130 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20717	20990	1.97	93.59
20990	20990	0.00	93.12
21816	21816	0.00	86.81
21919	21816	6.11	97.19

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Nicotinamide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20335-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Nicotinamide; Nicotinoylamidum

Special notes

When selecting the *Nicotinamide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Nicotinamide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Nicotinamide	13097506	21364	40	20130416
Euro OTC	Nicotinamide	1310025-01	21643	40	20131121
Euro OTC	Nicotinamide	1511010	22251	40	20151203*
Euro OTC	Nicotinamide	1601045	22374	40	20160210*
Euro OTC	Nicotinamide	1610019	22874	40	20161202*
Caelo	Nicotinamide	163048	23050	40	20161123*

Validation samples

A total of 280 317 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 *Nicotinamide*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 10 reference samples from the substance/substance group *Nicotinamide*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Nicotinamide	11001809	20647	40
Euro OTC	Nicotinamide	1310025-01	21643 [†]	20
Euro OTC	Nicotinamide	1511010	22251 [†]	20
Euro OTC	Nicotinamide	1601045	22374 [†]	20
Caelo	Nicotinamide	161136	22434	60
Caelo	Nicotinamide	161136	22625	40
Caelo	Nicotinamide	163048	23038	40
Euro OTC	Nicotinamide	1707001	23555	40
Caelo	Nicotinamide	173419	23785	40
Euro OTC	Nicotinamide	1801039	23957	40

- 126 532 spectra from a total of 2780 batches from further 781 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.

- 53 spectra from 29 *Apo-Ident* customers from 27 batches from the substance/substance group *Nicotinamide*.

Supplier	Substance	Batch	Spectra
Caelo	Nicotinamide	12268302	1
Noweda	Nicotinamide	12133403	2
DSM Nutritional Prod./ ...	Nicotinamide	1106044-01	1
Euro OTC	Nicotinamide	1108021-01	1
Caelo	Nicotinamide	12133403	1
Euro OTC	Nicotinamide	1211031-02	5
Fagron	Nicotinamide	12J02-B03	1
Caelo	Nicotinamide	13097504	1
Euro OTC	Nicotinamide	11208021	1
Fagron	Nicotinamide	L14020084	1
Caelo	Nicotinamide	13097506	1
Gatt-Koller	Nicotinamide	221406112411	1
Gatt-Koller	Nicotinamide	4456/10104110	1
Euro OTC	Nicotinamide	1310025-01	3
Phoenix	Nicotinamide	1211031-02	1
Caelo	Nicotinamide	13352002	1
VDL;16.04.15;5,60EUR	Nicotinamide	1408019-01	1
Euro OTC	Nicotinamide	131002501	1
Euro OTC	Nicotinamide	1408019-01	2
Caelo	Nicotinamide	14246806	1
Euro OTC	Nicotinamide	11401052	1
Euro OTC	Nicotinamide	1408019-19	1
Euro OTC	Nicotinamide	1503024-02	1
Caelo	Nicotinamide	1511010-01	1
Euro OTC	Nicotinamide	1601045-01	4
Euro OTC	Nicotinamide	1511010-01	3
Euro OTC	Nicotinamide	1610019-01	5
Caelo	Nicotinamide	16304803	1
Euro OTC	Nicotinamide	1707001-01	4
Caelo	Nicotinamide	1610019-01	1
Euro OTC	Nicotinamide		1
Euro OTC	Nicotinamide	1801039-01	2

- 78 876 spectra from 565 *Apo-Ident* customers from a total of 26 110 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Nicotinamide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nicotinamide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	360	0	126 532
Type C	0	53	0	78 876

The substance/substance group *Nicotinamide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 88.6792 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21364	22251	5.21	81.70
21643	22374	3.52	80.87
22251	22251	0.00	81.13
22374	22374	0.00	80.83
22874	22874	0.00	81.56
23050	23050	0.00	81.64

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Nicotinic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20383-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Nicotinic acid; Acidum nicotinicum

Special notes

When selecting the *Nicotinic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Nicotinic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Nicotinic acid	14E01-B09-293947	21692	40	AR-15-FG-008938-01
Fagron	Nicotinic acid	16H19-B02-330121	23225	40	AR-17-FG-016013-01

Validation samples

A total of 280 317 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 *Nicotinic acid*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Nicotinic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Nicotinic acid	14E01-B09-293947	21692 [†]	20
Euro OTC	Nicotinic acid	1801021	23954	40

- 126 832 spectra from a total of 2787 batches from further 781 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 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Nicotinic acid*.

Supplier	Substance	Batch	Spectra
gonmisol	Nicotinic acid	17-18/NCN(P)/B/008	1
Kehr	Nicotinic acid	1801021-01	2

[†]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*.

- 78 926 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Nicotinic 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 *Nicotinic 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	74 416
Type B	0	60	0	126 832
Type C	0	3	0	78 926

The substance/substance group *Nicotinic 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 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.8821 %)	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
21692	21692	0.00	58.72
23225	23225	0.00	56.73

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Non-ionic emulsifying alcohol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20467-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Non-ionic emulsifying alcohol; Alkoholes emulsificantes nonionici

Special notes

When selecting the *Non-ionic emulsifying alcohol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
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Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Non-ionic emulsifying alcohol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Non-ionic emulsi...	13413001	21069	40	1405257
apomix	Non-ionic emulsi...	NS-8350010216	23274	40	20160718

Validation samples

A total of 280317 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 *Non-ionic emulsifying alcohol*. These samples are listed above in the [calibration samples](#) section.
- 74416 spectra from a total of 1621 batches from further 372 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 *Non-ionic emulsifying alcohol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Non-ionic emulsifying alcohol	13413001	21524	40
Caelo	Non-ionic emulsifying alcohol	162231	22745	40
Caelo	Non-ionic emulsifying alcohol	171836	23576	40
Caelo	Non-ionic emulsifying alcohol	182021	24282	40

- 126732 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 41 spectra from 14 *Apo-Ident* customers from 15 batches from the substance/substance group *Non-ionic emulsifying alcohol*.

Supplier	Substance	Batch	Spectra
Bombastus	Non-ionic emulsifying alcohol	267575	2
Bombastus	Non-ionic emulsifying alcohol	274059	1
Bombastus	Non-ionic emulsifying alcohol	278281	4

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Supplier	Substance	Batch	Spectra
Phönix	Non-ionic emulsifying alcohol	274059	1
Caelo	Non-ionic emulsifying alcohol	21091302	1
Caelo	Non-ionic emulsifying alcohol	12254402	1
Bombastus	Non-ionic emulsifying alcohol	284009	2
Bombastus	Non-ionic emulsifying alcohol	292319	8
Caelo	Non-ionic emulsifying alcohol	14241503	1
Bombastus	Non-ionic emulsifying alcohol	295568	5
Caelo	Non-ionic emulsifying alcohol	15287902	3
Bombastus	Non-ionic emulsifying alcohol	2995568	1
Bombastus	Non-ionic emulsifying alcohol	304997	5
Bombastus	Non-ionic emulsifying alcohol	306666	4
Bombastus	Non-ionic emulsifying alcohol	3066	1
Bombastus	Non-ionic emulsifying alcohol	311625	1

- 78 888 spectra from 565 *Apo-Ident* customers from a total of 26 122 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Non-ionic emulsifying 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 *Non-ionic emulsifying 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	80	0	74 416
Type B	0	160	0	126 732
Type C	0	39	2	78 888

The substance/substance group *Non-ionic emulsifying 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 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	95.1220 % (> 87.8049 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21069	21069	0.00	31.18
23274	21069	9.66	33.82

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Norethisterone acetate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20797-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Norethisterone acetate; Norethisteroni acetat

Special notes

When selecting the *Norethisterone acetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Norethisterone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Norethisterone a...	12L14-N03	20797	40	1401558
Euro OTC	Norethisterone a...	1306033-01	21627	20	1511684
Caelo	Norethisterone a...	15417004	23122	40	1711489
Caelo	Norethisterone a...	182252	24395	40	20181031*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 4 reference samples from the substance/substance group *Norethisterone acetate*. These samples are listed above in the [calibration samples](#) section.
- 74 356 spectra from a total of 1619 batches from further 372 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 *Norethisterone acetate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Norethisterone acetate	1306033-01	21627 [†]	40
Fagron	Norethisterone acetate	14H29-B03-325225	23171	40
Fagron	Norethisterone acetate	17B21-B01-341608	23918	40

- 126 772 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 19 spectra from 14 *Apo-Ident* customers from 16 batches from the substance/substance group *Norethisterone acetate*.

*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
Fagron	Norethisterone acetate	22061206	1
Fagron	Norethisterone acetate	12C06-N10	2
Bombastus	Norethisterone acetate	13J08-N04	1
Fagron	Norethisterone acetate	13J08-N04	1
Fagron	Norethisterone acetate	14H29-B03-299313	1
Fagron	Norethisterone acetate	14h29-b03-310697	1
Fagron	Norethisterone acetate	14D08-B01-292738	1
Euro OTC	Norethisterone acetate	1306033-02	2
Fagron	Norethisterone acetate	14d08-b01-292736	1
Euro/Phönix	Norethisterone acetate	1306033-01	1
Fagron	Norethisterone acetate	14H29-B03-321322	1
Fagron	Norethisterone acetate	13D19-N06	1
Fagron	Norethisterone acetate	14H29-B03-325224	1
Caelo	Norethisterone acetate	15417008	1
Fagron	Norethisterone acetate	17B21-B01	1
Caelo	Norethisterone acetate	15417001	1
Fagron	Norethisterone acetate	17B21-B01-341608	1

- 78 910 spectra from 565 *Apo-Ident* customers from a total of 26 121 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Norethisterone 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 *Norethisterone 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	140	0	74 356
Type B	0	120	0	126 772
Type C	0	19	0	78 910

The substance/substance group *Norethisterone 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 % (> 99.9887 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
23122	23122	0.00	9.54
21627	21627	0.00	11.21
20797	20797	0.00	12.65
24395	24395	0.00	14.00

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Nystatin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20116-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Nystatin; Nystatinum

Special notes

When selecting the *Nystatin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Nystatin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Nystatin	16272214	23711	40	20160929
Euro OTC	Nystatin	1712010-01	24103	40	1807445

Validation samples

A total of 280 317 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 *Nystatin*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Nystatin*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Nystatin	16L21-B01-338864	23712	40
Euro OTC	Nystatin	1612001-03	23727	40
Caelo	Nystatin	17025110	23984	40
Audor Pharma	Nystatin	AP4018717N	23985	40

- 126 732 spectra from a total of 2785 batches from further 781 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.

- 186 spectra from 112 *Apo-Ident* customers from 76 batches from the substance/substance group *Nystatin*.

Supplier	Substance	Batch	Spectra
Caelo	Nystatin	11069706	2
Fagron	Nystatin	11C21-N10	1
Euro OTC	Nystatin	1107036-01	4

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Supplier	Substance	Batch	Spectra
Caelo	Nystatin	11069731	1
Euro OTC	Nystatin	1107046-01	2
Phönix	Nystatin	12017005	2
Anzag	Nystatin	2902041-02	1
Caelo	Nystatin	11069716	1
Caelo	Nystatin	11069719	1
Caelo	Nystatin	12017004	3
Caelo	Nystatin	11069730	1
Caesar&loretz,Phoenix	Nystatin	1111057-01	3
Euro OTC	Nystatin		1
Caelo	Nystatin	12017009	1
Caelo	Nystatin	3101201	1
Euro OTC	Nystatin	1111057-01	3
Euro OTC	Nystatin	4014991	1
Caelo	Nystatin	C129330	1
Caelo	Nystatin	13101201	1
Caelo	Nystatin	13101202	1
EuRho	Nystatin	1107046-01	1
Caelo	Nystatin	1107046-01	1
Caelo	Nystatin	12017003	1
Gehe	Nystatin	1207009-01	1
Caelo	Nystatin	11069704	1
Fagron	Nystatin	11K11-No4	1
Noweda	Nystatin	1207009-01	1
Fagron	Nystatin	20121202	1
Sanacorp	Nystatin	1107046-01	1
Caelo	Nystatin	12017011	2
Caelo	Nystatin	12158006	7
Phönix/Euro	Nystatin	1111057-01	1
Euro OTC	Nystatin	1207009-01	6
EuRho/Anzag	Nystatin	1107036-01	1
Caelo	Nystatin	12017010	1
Gehe	Nystatin	1107036-01	1
Europharm/Otto	Nystatin	1107046-01	1
Gehe	Nystatin	1111057-01	1
Caelo	Nystatin	12158004	3
Euro OTC	Nystatin	1207009-02	2
Fagron	Nystatin	4014376	1
Caelo	Nystatin	12158004	1
DSM Caiua S.p.A	Nystatin	1207009-01	1
Euro OTC	Nystatin	C129440	1
Fagron	Nystatin	12G04-N12	1
Euro OTC	Nystatin	C129531	2
Euro OTC	Nystatin	1212024-01	14
Caesar&loretz,Anzag	Nystatin	12158008	3
Caelo	Nystatin	12017015	2
Caelo	Nystatin	12158008	3
Caelo	Nystatin	12158019	3
Caelo	Nystatin	12158010	3
Caelo	Nystatin	12158005	1
Caelo	Nystatin	6082013B	1
Phönix	Nystatin	1212024-01	1
EuRho	Nystatin	1207009-01	1
Euro OTC	Nystatin	127009-02	1
Caelo	Nystatin	12158009	1
Caelo	Nystatin	2091304	1
Euro OTC	Nystatin	1212024-02	13
Fagron	Nystatin	12C29-N09	1
Gehe	Nystatin	12158008	1
Fagron	Nystatin	13C11-N08	1

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Supplier	Substance	Batch	Spectra
Caelo	Nystatin	12158020	1
Caelo	Nystatin	13173401	7
Caesar&lorenz,Phoenix	Nystatin	1218008	1
Caesar&lorenz,Phoenix	Nystatin	13173401	4
Caelo	Nystatin	12158021	2
Euro OTC	Nystatin	2811032-01	1
Sanacorp	Nystatin	1212024-02	1
Phönix	Nystatin	1212024-02	1
Euro OTC	Nystatin	1307053-01	5
Caelo	Nystatin	12138021	2
Phönix	Nystatin	12158010	1
Caelo	Nystatin	12158022	1
EUro/AHD	Nystatin	1307053-01	1
Euro OTC	Nystatin	121024-01	1
Caelo	Nystatin	121580921	1
Caesar&lorenz,Phoenix	Nystatin	13173408	1
Euro OTC	Nystatin	130705301	1
Caelo	Nystatin	13173408	1
Euro OTC	Nystatin	1307053-02	2
Caesar&lorenz,AHC	Nystatin	14196509	2
Caelo	Nystatin	15335310	1
Euro OTC	Nystatin	C129854	1
Euro OTC	Nystatin	1511020-01	1
Euro OTC	Nystatin	1511020-02	1
Caelo	Nystatin	14363514	1
Gehe	Nystatin	1307053-02	1
Euro OTC	Nystatin	1712010-01	5
Caesar&lorenz,Phoenix	Nystatin	14363512	1
Caelo	Nystatin	1712010-01	2
Caelo	Nystatin	18072109	2
Caelo	Nystatin	18072108	1
Caelo	Nystatin	18072014	1
Caelo	Nystatin	18072105	1
Euro OTC	Nystatin	16120001-02	1
Caelo	Nystatin	18072114	1
Kehr	Nystatin	1612001-02	1
Anzag	Nystatin	1712010-01	1
Caelo	Nystatin	18072121	1

- 78 743 spectra from 565 *Apo-Ident* customers from a total of 26 062 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Nystatin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nystatin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	160	0	126 732
Type C	0	52	134	78 743

The substance/substance group *Nystatin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	27.9570 % (> 26.3441 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
23711	24103	4.28	16.23
24103	24103	0.00	15.91

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Octenidine dihydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20759-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Octenidine dihydrochloride; Octenidini dihydrochloridum

Special notes

When selecting the *Octenidine dihydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Octenidine dihydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Octenidine dihyd...	12115202	20759	40	20120511
Caelo	Octenidine dihyd...	13071407	20988	40	1407345
Caelo	Octenidine dihyd...	13166806	21331	40	20130718
Caelo	Octenidine dihyd...	15275502	21888	40	20150910
Caelo	Octenidine dihyd...	15356601	21947	40	1604116

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Octenidine dihyd...	170423	23307	40	20170214*
Caelo	Octenidine dihyd...	163355	23309	40	20170403*
Caelo	Octenidine dihyd...	15356601	21947SI	40	1604116
Caelo	Octenidine dihyd...	170423	23307SI	40	20170214*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Octenidine dihydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 136 spectra from a total of 1616 batches from further 372 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 8 reference samples from the substance/substance group *Octenidine dihydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Octenidine dihydrochloride	15275502	21888 [†]	20
Caelo	Octenidine dihydrochloride	15356601	21947 [†]	20
Caelo	Octenidine dihydrochloride	160330	22485	60
Caelo	Octenidine dihydrochloride	180174	24023	40
Caelo	Octenidine dihydrochloride	15275502	21888SI	60
Caelo	Octenidine dihydrochloride	15356601	21947SI [†]	20
Caelo	Octenidine dihydrochloride	163355	23309SI	40
Caelo	Octenidine dihydrochloride	180174	24023SI	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*.

- 126 592 spectra from a total of 2784 batches from further 781 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.

- 277 spectra from 151 *Apo-Ident* customers from 72 batches from the substance/substance group *Octenidine dihydrochloride*.

Supplier	Substance	Batch	Spectra
Caelo	Octenidine dihydrochloride	13166801	1
Caelo	Octenidine dihydrochloride	13166808	2
Caelo	Octenidine dihydrochloride	13166810	1
Caelo	Octenidine dihydrochloride	15006202	3
Apomix/Noweda	Octenidine dihydrochloride	13166813	1
Caelo	Octenidine dihydrochloride	15006203	1
Löwen City-Apotheke Bar...	Octenidine dihydrochloride	2042015	1
Cealo/Sanacorp	Octenidine dihydrochloride	15006207	1
Caelo	Octenidine dihydrochloride	15006207	5
Fresenius	Octenidine dihydrochloride	60715101	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	15006210	1
Caelo	Octenidine dihydrochloride	15275503	2
Caelo	Octenidine dihydrochloride	15275504	1
Caelo	Octenidine dihydrochloride	15275502	5
Caelo	Octenidine dihydrochloride	15356601	6
Caelo	Octenidine dihydrochloride	15356603	3
Caelo	Octenidine dihydrochloride	15356703	6
Caelo	Octenidine dihydrochloride	1515E-03732	1
Fagron	Octenidine dihydrochloride	15356703	1
Caelo	Octenidine dihydrochloride	16032803	6
Caelo	Octenidine dihydrochloride	16032902	4
Caelo	Octenidine dihydrochloride	16032903	1
Euro OTC	Octenidine dihydrochloride	16032803	1
Caelo	Octenidine dihydrochloride	152755020	1
Caelo	Octenidine dihydrochloride	16032909	6
Caelo	Octenidine dihydrochloride	16033002	2
Caelo	Octenidine dihydrochloride	16032901	1
Caelo	Octenidine dihydrochloride	16033001	2
Caelo	Octenidine dihydrochloride	16032910	3
Celo	Octenidine dihydrochloride	16277802	1
Caelo	Octenidine dihydrochloride	16277802	7
Fagron	Octenidine dihydrochloride	16277802	1
Caelo	Octenidine dihydrochloride	16325304	7
GEHE	Octenidine dihydrochloride	16325304	1
Caelo	Octenidine dihydrochloride	16302910	1
Caelo	Octenidine dihydrochloride	816M-03732	1
Caelo	Octenidine dihydrochloride	16325406	5
Caelo	Octenidine dihydrochloride	6325305	1
Cealo/Sanacorp	Octenidine dihydrochloride	16325305	1
Caelo	Octenidine dihydrochloride	16325305	6
Caelo	Octenidine dihydrochloride	17042602	6
GEHE	Octenidine dihydrochloride	16325305	1
Caelo	Octenidine dihydrochloride	17042302	5
Caelo	Octenidine dihydrochloride	17042305	3
Caelo	Octenidine dihydrochloride	17042304	9

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Supplier	Substance	Batch	Spectra
Caelo	Octenidine dihydrochloride	16325408	2
Caelo	Octenidine dihydrochloride	17042903	13
Caelo	Octenidine dihydrochloride	17042303	1
Anzag	Octenidine dihydrochloride	17042602	1
Caelo	Octenidine dihydrochloride	16335502	2
Caesar&Loretz GmbH, 14...	Octenidine dihydrochloride	17042302	1
Caelo	Octenidine dihydrochloride	16335505	3
Caelo	Octenidine dihydrochloride	16325410	1
Caelo	Octenidine dihydrochloride	16335504	10
Caesar&Loretz GmbH	Octenidine dihydrochloride	16335504	1
Sanacorp	Octenidine dihydrochloride	16335504	1
Caelo	Octenidine dihydrochloride	16335509	4
Caelo	Octenidine dihydrochloride	16335508	2
Caelo	Octenidine dihydrochloride	1711160HC/16335509	1
Caelo	Octenidine dihydrochloride	172118501	1
Noweda	Octenidine dihydrochloride	16335507	1
Caelo	Octenidine dihydrochloride	17218501	10
Caelo	Octenidine dihydrochloride	16335510	1
Caelo	Octenidine dihydrochloride	16335507	3
Caelo	Octenidine dihydrochloride	17218506	10
Caelo	Octenidine dihydrochloride	17042501	1
Caelo	Octenidine dihydrochloride	172185035514	1
Caelo	Octenidine dihydrochloride	17218508	7
Caelo	Octenidine dihydrochloride	17218503	6
Caelo	Octenidine dihydrochloride	1728506	1
Caelo	Octenidine dihydrochloride	16335506	1
Caelo	Octenidine dihydrochloride	17218507	5
Jenne	Octenidine dihydrochloride	17218507	1
Hepart	Octenidine dihydrochloride	17218508	1
Kehr	Octenidine dihydrochloride	17218508	1
Caelo	Octenidine dihydrochloride	11071925	1
Caelo	Octenidine dihydrochloride	18017402	18
Caelo	Octenidine dihydrochloride	13061801	1
Caesar & Lorenz GmbH	Octenidine dihydrochloride	17218503	1
Caelo	Octenidine dihydrochloride	17218509	10
Caelo	Octenidine dihydrochloride	300718A	1
Caelo	Octenidine dihydrochloride	17218507	1
Caelo	Octenidine dihydrochloride	18197501	10
Caesar & Loretz GmbH	Octenidine dihydrochloride	181975002	1
Caelo	Octenidine dihydrochloride	181975025789	1
Caelo	Octenidine dihydrochloride	18197502	1
Caelo	Octenidine dihydrochloride	18223403	5
Caelo	Octenidine dihydrochloride	18197504	2
Gehe 21-01-2019	Octenidine dihydrochloride	18223403	1
Caelo	Octenidine dihydrochloride	18223409	2
Caelo	Octenidine dihydrochloride	18223404	1

- 78 652 spectra from 565 *Apo-Ident* customers from a total of 26 066 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Octenidine dihydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this

purpose, all relevant spectra of the various substances were compared with *Octenidine dihydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	74 136
Type B	0	300	0	126 592
Type C	0	268	9	78 652

The substance/substance group *Octenidine dihydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.8817 %)	96.7509 % (> 95.6679 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20759	23309	4.72	29.52
20988	20988	0.00	30.34
21331	21947	7.89	32.43
23309	23309	0.00	28.77
23307	23307	0.00	31.46
21888	21947	4.39	45.24
21947	21947	0.00	39.78

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ofloxacin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21047-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ofloxacin; Ofloxacinum

Special notes

When selecting the *Ofloxacin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Ofloxacin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ofloxacin	13A17-N01	21047	40	1403155
Fagron	Ofloxacin	15H19-B01-312926	21918	40	20151006
Fagron	Ofloxacin	15H19-B01-325226	23090	40	1707611

Validation samples

A total of 280 317 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 *Ofloxacin*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 [†].

- 430 spectra of 10 reference samples from the substance/substance group *Ofloxacin*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ofloxacin	13A17-N01	21052	40
Fagron	Ofloxacin	13A17-N01	21811	60
Fagron	Ofloxacin	15H19-B01-312926	21918 [†]	20
Fagron	Ofloxacin	15H19-B01-337265	23753	40
Fagron	Ofloxacin	15H19-B01-337265	23754	40
Fagron	Ofloxacin	13A17-N01	21811SI	60
Fagron	Ofloxacin	15H19-B01-312926	21918SI	60
Fagron	Ofloxacin	15H19-B01-325226	23090SI	30
Fagron	Ofloxacin	15H19-B01-337265	23753SI	40
Fagron	Ofloxacin	15H19-B01-337265	23754SI	40

- 126 462 spectra from a total of 2785 batches from further 781 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*.

- 4 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Ofloxacin*.

Supplier	Substance	Batch	Spectra
Fagron	Ofloxacin	13A17-N01	2
Fagron	Ofloxacin	15H19-B01-314470	1
Caelo	Ofloxacin	15H19-B01	1

- 78 925 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ofloxacin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ofloxacin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	422	8	126 462
Type C	0	4	0	78 925

The substance/substance group *Ofloxacin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	98.1395 % (> 97.4419 %)
Type C	100.0000 % (> 99.8820 %)	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
21047	21047	0.00	23.69
21918	23090	7.64	29.83
23090	23090	0.00	20.95

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Omeprazole**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21098-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Omeprazole; Omeprazolum

Special notes

When selecting the *Omeprazole* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Omeprazole*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Inresa	Omeprazole	0PFP14017	21787	40	1507407
Fagron	Omeprazole	15K12-B02-314608	22890	40	20151124
Inresa	Omeprazole	0PFP14017	23273	40	20150428

Validation samples

A total of 280 317 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 *Omeprazole*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1621 batches from further 372 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 *Omeprazole*.

Supplier	Substance	Batch	Sample ID	Spectra
Inresa	Omeprazole	OPFP14017	21787 [†]	20
Inresa	Omeprazole	OPFP14017	21796	60
Inresa	Omeprazole	OPFP14017	22284	60
Fagron	Omeprazole	15K12-B02-314608	22740	40
Fagron	Omeprazole	16I20-B03-328940	23272	40

- 126 672 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 20 spectra from 15 *Apo-Ident* customers from 11 batches from the substance/substance group *Omeprazole*.

[†]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
Fagron	Omeprazole	15B26-B40-305669	2
Fagron	Omeprazole	15K12-B02-314608	3
Fagron	Omeprazole	15K12-B02	1
Fagron	Omeprazole	15K12-B02-525174	2
Fagron	Omeprazole	15k12-B02	1
Fagron	Omeprazole	16B16-B01-52535	1
Fagron	Omeprazole	16/20-B03-328940	3
Fagron	Omeprazole	0PFP16030	1
Fagron	Omeprazole	16120-B03-328940	1
Sanacorp	Omeprazole	17H15-B03-342821	1
Fagron	Omeprazole	17H15-B03-342821	1
Fagron	Omeprazole	17K28-B07-348698	3

- 78 909 spectra from 565 *Apo-Ident* customers from a total of 26 126 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Omeprazole* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Omeprazole* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	220	0	126 672
Type C	0	19	1	78 909

The substance/substance group *Omeprazole* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.8817 %)	95.0000 % (> 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
21787	21787	0.00	57.99
22890	21787	6.42	61.01
23273	21787	4.12	63.99

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ornithine aspartate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20842-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ornithine aspartate; Ornithinum asparticum

Special notes

When selecting the *Ornithine aspartate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Ornithine aspartate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ornithine aspart...	L1304034-01	20842	40	1402571
Fagron	Ornithine aspart...	14A20-B07-296093	21694	30	1506279
Euro OTC	Ornithine aspart...	1312030-01	21710	40	1506280
Fagron	Ornithine aspart...	14I24-B04-307758	22600	40	20141110
Euro OTC	Ornithine aspart...	1611018	22924	40	20161213*
Euro OTC	Ornithine aspart...	1611018-01	23198	40	20161213
Fagron	Ornithine aspart...	17I21-B05-342561	23864	40	1804455

Validation samples

A total of 280317 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 *Ornithine aspartate*. These samples are listed above in the [calibration samples](#) section.
- 74226 spectra from a total of 1616 batches from further 372 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 *Ornithine aspartate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ornithine aspartate	14A20-B07-296093	21694 [†]	15
Euro OTC	Ornithine aspartate	1312030-01	21710 [†]	20
Fagron	Ornithine aspartate	14I24-B04-307758	22599	40
Euro OTC	Ornithine aspartate	1711015	23899	40
Euro OTC	Ornithine aspartate	1805026	24125	40

- 126737 spectra from a total of 2784 batches from further 781 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*.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ornithine aspartate*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ornithine aspartate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ornithine aspartate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 226
Type B	0	155	0	126 737
Type C	0	0	0	78 929

The substance/substance group *Ornithine aspartate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.1290 %)
Type C	100.0000 % (> 99.8817 %)	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
22924	22924	0.00	66.18
22600	21710	2.82	57.87
20842	20842	0.00	57.46
23864	23864	0.00	49.69
21710	21710	0.00	58.45
21694	21694	0.00	66.77
23198	21694	9.08	75.31

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ornithine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20389-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ornithine hydrochloride; Ornithinum hydrochloricum

Special notes

When selecting the *Ornithine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Ornithine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ornithine hydroc...	13A03-N05	20967	40	1403094
Euro OTC	Ornithine hydroc...	1307028-01	21622	80	20130813
Euro OTC	Ornithine hydroc...	1605011	22573	40	20160601*

Validation samples

A total of 280 317 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 *Ornithine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1620 batches from further 372 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 *Ornithine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ornithine hydrochloride	1307028-01	21622 [†]	40
Euro OTC	Ornithine hydrochloride	1612009	22923	40
Euro OTC	Ornithine hydrochloride	1612009-01	23009	40
Euro OTC	Ornithine hydrochloride	1704006	23159	40
Euro OTC	Ornithine hydrochloride	1803018	24085	40

- 126 692 spectra from a total of 2784 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 7 spectra from 3 *Apo-Ident* customers from 7 batches from the substance/substance group *Ornithine hydrochloride*.

*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
Fagron	Ornithine hydrochloride	13A03-N05	1
Euro OTC	Ornithine hydrochloride	4712A-03475	1
Euro OTC	Ornithine hydrochloride	1014I-03475	1
Fagron	Ornithine hydrochloride	15A13-B03	1
Euro OTC	Ornithine hydrochloride	315E-03475	1
Euro OTC	Ornithine hydrochloride	516Q-03475	1
Euro OTC	Ornithine hydrochloride	1704006-01	1

- 78 922 spectra from 565 *Apo-Ident* customers from a total of 26 130 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ornithine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ornithine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	200	0	126 692
Type C	0	7	0	78 922

The substance/substance group *Ornithine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8818 %)	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
22573	22573	0.00	66.93
20967	20967	0.00	66.73
21622	22573	2.24	67.31

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Oxalic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20458-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Oxalic acid; Acidum oxalicum cryst.

Special notes

When selecting the *Oxalic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Oxalic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Oxalic acid	13353901	21042	40	20131029
Caelo	Oxalic acid	12212410	21066	40	1403223
Caelo	Oxalic acid	13353918	21774	40	20131029
Caelo	Oxalic acid	171140	23688	40	20170426*

Validation samples

A total of 280 317 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 *Oxalic acid*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Oxalic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oxalic acid	13353905	21453	60
Caelo	Oxalic acid	13353918	21774 [†]	20
Caelo	Oxalic acid	171140	23287	40
Caelo	Oxalic acid	18202403	24428	40

- 126 732 spectra from a total of 2785 batches from further 781 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*.

- 25 spectra from 20 *Apo-Ident* customers from 23 batches from the substance/substance group *Oxalic acid*.

Supplier	Substance	Batch	Spectra
Caelo	Oxalic acid	12212407	1
Caelo	Oxalic acid	12212406	1
Caelo	Oxalic acid	12212411	1
Caelo	Oxalic acid	12147010	1
Nachprüfung sanacorp	Oxalic acid		1
	Oxalic acid	11098213	1
Caelo	Oxalic acid	4812U-01039	1
Caelo	Oxalic acid	13353901	1
Caelo	Oxalic acid	13353907	2
Caelo	Oxalic acid	13353905	2
Caelo	Oxalic acid	13195413	1
Caelo	Oxalic acid	13353910	1
Caelo	Oxalic acid	914E-01039	1
Caelo	Oxalic acid	14334703	1
Caelo	Oxalic acid	13353915	1
Caesar&Loretz GmbH/ All...	Oxalic acid	13353920	1
Caelo	Oxalic acid	10383104	1
Caelo	Oxalic acid	11111703	1
Caelo	Oxalic acid	13195414	1
Caelo	Oxalic acid	16297401	1
Caelo	Oxalic acid	17114003	1
Caelo	Oxalic acid	16050205	1
Caelo	Oxalic acid	7111808	1

- 78 904 spectra from 565 *Apo-Ident* customers from a total of 26 115 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Oxalic 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 *Oxalic 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	154	6	74 336
Type B	0	120	40	126 732
Type C	0	16	9	78 904

The substance/substance group *Oxalic 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 % (> 99.9887 %)	96.2500 % (> 94.3750 %)
Type B	100.0000 % (> 99.9901 %)	75.0000 % (> 73.1250 %)
Type C	100.0000 % (> 99.8817 %)	64.0000 % (> 52.0000 %)

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
21042	21066	4.15	64.99
21066	21066	0.00	72.27
21774	21066	3.30	67.43
23688	23688	0.00	72.14

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Oxetacaine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 23686-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Oxetacaine; Oxetacainum

Special notes

When selecting the *Oxetacaine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Oxetacaine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Oxetacaine	172498	23686	40	20170925*
Audor	Oxetacaine	AP010-160120	24104	40	1809415

Validation samples

A total of 280 317 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 *Oxetacaine*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Oxetacaine*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oxetacaine	17249805	23916	50

- 126 842 spectra from a total of 2788 batches from further 781 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 *Oxetacaine*.

Supplier	Substance	Batch	Spectra
Caelo	Oxetacaine	17249810	1
Kehr	Oxetacaine	17249805	1

*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.

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Oxetacaine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxetacaine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	50	0	126 842
Type C	0	2	0	78 927

The substance/substance group *Oxetacaine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 88.0000 %)
Type C	100.0000 % (> 99.8823 %)	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
23686	23686	0.00	25.90
24104	24104	0.00	23.97

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Oxybuprocaine hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20958-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Oxybuprocaine hydrochloride; Oxybuprocaini hydrochloridum

Special notes

When selecting the *Oxybuprocaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
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Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Oxybuprocaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Oxybuprocaine hy...	13D16-N12	20958	40	1402060
Fagron	Oxybuprocaine hy...	13J24-B07-295015	21799	40	AR-15-FG-014812-02
Fagron	Oxybuprocaine hy...	15A26-B07-306787	21922	40	20150203
Fagron	Oxybuprocaine hy...	17G21-B03-338576	23745	40	20170823

Validation samples

A total of 280 317 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 *Oxybuprocaine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 [†].

- 280 spectra of 7 reference samples from the substance/substance group *Oxybuprocaine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Oxybuprocaine hydrochloride	13J24-B07-295015	21799 [†]	20
Fagron	Oxybuprocaine hydrochloride	15A26-B07-306787	21922 [†]	20
Fagron	Oxybuprocaine hydrochloride	16L05-B06-334330	23719	40
Fagron	Oxybuprocaine hydrochloride	16L05-B06-334330	23720	40
Fagron	Oxybuprocaine hydrochloride	16L05-B06-334330	23752	40
Fagron	Oxybuprocaine hydrochloride	13J24-B07-295015	21799SI	60
Fagron	Oxybuprocaine hydrochloride	15A26-B07-306787	21922SI	60

- 126 612 spectra from a total of 2786 batches from further 781 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*.

- 13 spectra from 7 *Apo-Ident* customers from 9 batches from the substance/substance group *Oxybuprocaine hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	Oxybuprocaine hydrochloride	12L19N01	1
Fagron	Oxybuprocaine hydrochloride	13C01-N01	4
Fagron	Oxybuprocaine hydrochloride	4612M-03639	1
Klenk	Oxybuprocaine hydrochloride	3613M-07321	1
Fagron	Oxybuprocaine hydrochloride	3613N-07321	1
Fagron	Oxybuprocaine hydrochloride	13h13-n05	2
Fagron	Oxybuprocaine hydrochloride	13J24B07295015	1
Caelo	Oxybuprocaine hydrochloride	14G21B02300384	1
Fagron	Oxybuprocaine hydrochloride	15A26-B07	1

- 78 916 spectra from 565 *Apo-Ident* customers from a total of 26 128 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Oxybuprocaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxybuprocaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	266	14	126 612
Type C	0	12	1	78 916

The substance/substance group *Oxybuprocaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	95.0000 % (> 93.9286 %)
Type C	100.0000 % (> 99.8818 %)	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
21799	21799	0.00	41.75
20958	20958	0.00	53.15
21922	21799	10.44	50.17
23745	20958	8.58	52.31

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Oxybutynin hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20565-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Oxybutynin hydrochloride; Oxybutynini hydrochloridum

Special notes

When selecting the *Oxybutynin hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Oxybutynin hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Oxybutynin hydro...	13H26-B03-290572	21543	40	AR-15-FG-002173-01
Fagron	Oxybutynin hydro...	14A29-B09-293841	21704	30	20140227
Fagron	Oxybutynin hydro...	14I16-B03-312059	22732	40	20141007

Validation samples

A total of 280317 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 *Oxybutynin hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74386 spectra from a total of 1620 batches from further 372 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 *Oxybutynin hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Oxybutynin hydrochloride	12D24-N07	20565	40
Fagron	Oxybutynin hydrochloride	13H26-B03-290572	21543 [†]	20
Fagron	Oxybutynin hydrochloride	14A29-B09-293841	21704 [†]	15
Fagron	Oxybutynin hydrochloride	16A18-B02-321181	23268	40
Fagron	Oxybutynin hydrochloride	18A12-B03-344347	23995	40

- 126737 spectra from a total of 2784 batches from further 781 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.

- 65 spectra from 15 *Apo-Ident* customers from 34 batches from the substance/substance group *Oxybutynin hydrochloride*.

[†]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
Fagron	Oxybutynin hydrochloride	13H26-B03-287325	1
Fagron	Oxybutynin hydrochloride	14a29-b09-307322	2
Fagron	Oxybutynin hydrochloride	14A29-B09-307322	1
Fagron	Oxybutynin hydrochloride	13H26-B03	1
Caelo	Oxybutynin hydrochloride	14A29-B09-307322	4
Fagron	Oxybutynin hydrochloride	14/16-B03-300207	4
Fagron	Oxybutynin hydrochloride	127979	1
Fagron	Oxybutynin hydrochloride	14/16B03300207	1
Fagron	Oxybutynin hydrochloride	14A29B09307322	2
Fagron	Oxybutynin hydrochloride	15F05-B03-315221	5
Fagron	Oxybutynin hydrochloride	15F05-b03-315220	1
Caelo	Oxybutynin hydrochloride	15F05B03315221	5
Caelo	Oxybutynin hydrochloride	15F05-B03-318524	4
Fagron	Oxybutynin hydrochloride	14I16-B03-300207	1
Fagron	Oxybutynin hydrochloride	1607080	1
Caelo	Oxybutynin hydrochloride	129099	1
Fagron	Oxybutynin hydrochloride	16A18-B02-322538	3
Fagron	Oxybutynin hydrochloride	129099	1
Fagron	Oxybutynin hydrochloride	14/16-B03-300209	1
Caelo	Oxybutynin hydrochloride	16A18-B02-321181	3
Fagron	Oxybutynin hydrochloride	14I16-B03	1
Fagron	Oxybutynin hydrochloride	16A18-B02-326183	1
Fagron	Oxybutynin hydrochloride	16I23-B03-328916	2
Fagro/Sanacorp	Oxybutynin hydrochloride	16A18-B02-326183	1
Caelo	Oxybutynin hydrochloride	16A18B02321181	2
Fagron	Oxybutynin hydrochloride	16/23-b03-333371	1
Fagron	Oxybutynin hydrochloride	1709250/16I23-B03-33	1
Fagro/Sanacorp	Oxybutynin hydrochloride	16/23-B03-32891613	1
Fagron	Oxybutynin hydrochloride	16I23-b03-328916	1
Caelo	Oxybutynin hydrochloride	16/23-B03-333371	3
Caelo	Oxybutynin hydrochloride	16A18-B02-326183	1
Caelo	Oxybutynin hydrochloride	16/23-B03-328916	1
Caelo	Oxybutynin hydrochloride	18A12-Bo3-344350	1
Fagron	Oxybutynin hydrochloride	18A12-B03-344347	1
Fagron	Oxybutynin hydrochloride	18A12-B03-344348	1
Caelo	Oxybutynin hydrochloride	18A12-B03-344350	1
Audor Pharma	Oxybutynin hydrochloride	AP0H0122017-2018-10B	1
Fagron	Oxybutynin hydrochloride	18A12-B03-346964	1

- 78 864 spectra from 565 *Apo-Ident* customers from a total of 26 103 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Oxybutynin hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxybutynin hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 386
Type B	0	155	0	126 737
Type C	0	59	6	78 864

The substance/substance group *Oxybutynin hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 94.5455 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.1290 %)
Type C	100.0000 % (> 99.8817 %)	90.7692 % (> 86.1538 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21543	21543	0.00	34.86
22732	21543	3.32	34.86
21704	21543	4.21	33.34

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Oxytetracycline hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20090-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Oxytetracycline hydrochloride; Oxytetracyclini hydrochloridum

Special notes

When selecting the *Oxytetracycline hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Oxytetracycline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Oxytetracycline ...	12130001	20847	40	20120530
Fagron	Oxytetracycline ...	13D08-N11	20848	60	20110131
Caelo	Oxytetracycline ...	12328103	21039	40	20121214
Euro OTC	Oxytetracycline ...	1306022-02	21600	40	1507542
Euro OTC	Oxytetracycline ...	1506037	21836	40	20150721*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Oxytetracycline ...	15D29-B99-309066	21915	40	20150522
Euro OTC	Oxytetracycline ...	1506037	21999	40	20150721*
Caelo	Oxytetracycline ...	16077002	22503	40	AR-16-FG-011460-01
Euro OTC	Oxytetracycline ...	1602025	22546	40	20160609*
Euro OTC	Oxytetracycline ...	1602025-01	22658	40	AR-16-FG-014422-01
Euro OTC	Oxytetracycline ...	1602025	22669	40	20160609*
Euro OTC	Oxytetracycline ...	1602025-02	22839	40	20161021
Euro OTC	Oxytetracycline ...	1701034	23137	40	20170314*
Euro OTC	Oxytetracycline ...	1701035-02	23970	40	20170314

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 580 spectra of 14 reference samples from the substance/substance group *Oxytetracycline hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 73916 spectra from a total of 1611 batches from further 372 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 *Oxytetracycline hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oxytetracycline hydrochloride	12130001	20847 [†]	20
Euro OTC	Oxytetracycline hydrochloride	1306022-02	21600 [†]	20
Euro OTC	Oxytetracycline hydrochloride	1506037	21836 [†]	20
Fagron	Oxytetracycline hydrochloride	15D29-B99-309066	21915 [†]	20
Euro OTC	Oxytetracycline hydrochloride	1506037	21999 [†]	20
Euro OTC	Oxytetracycline hydrochloride	1602025-02	22846	40
Fagron	Oxytetracycline hydrochloride	15L16-B02-322908	23226	40
Fagron	Oxytetracycline hydrochloride	15L16-B02-322908	23417	40
Caelo	Oxytetracycline hydrochloride	173168	23786	40
Euro OTC	Oxytetracycline hydrochloride	1801033	23971	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.

- 126 592 spectra from a total of 2781 batches from further 781 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.

- 448 spectra from 187 *Apo-Ident* customers from 112 batches from the substance/substance group *Oxytetracycline hydrochloride*.

Supplier	Substance	Batch	Spectra
Euro OTC	Oxytetracycline hydrochloride	1111061-01	6
Fagron	Oxytetracycline hydrochloride	C22H25CIN209	1
Fagron	Oxytetracycline hydrochloride	12A26-N05	2
Gehe	Oxytetracycline hydrochloride	12A26-N05	2
Caelo	Oxytetracycline hydrochloride	11336510	2
Euro OTC	Oxytetracycline hydrochloride	1111061-61	1
Euro OTC	Oxytetracycline hydrochloride	1011045-01	3
Euro OTC	Oxytetracycline hydrochloride	1205028-01	6
Fagron	Oxytetracycline hydrochloride	12G10-N04	7
EuRho	Oxytetracycline hydrochloride	1111061-01	1
Caelo	Oxytetracycline hydrochloride	12G10-N04	1
Caelo	Oxytetracycline hydrochloride	21021305	1
Euro OTC	Oxytetracycline hydrochloride	513E-02865	1
Phönix	Oxytetracycline hydrochloride	1205028-01	1
EuRho	Oxytetracycline hydrochloride	1205028-01	2
Alliance Healthcare	Oxytetracycline hydrochloride	1205222-01	1
Caelo	Oxytetracycline hydrochloride	11336507	1
Gehe	Oxytetracycline hydrochloride	12g10-n04	1
Alliance Healthcare	Oxytetracycline hydrochloride	1205028-02	1
Euro OTC	Oxytetracycline hydrochloride	1205028-02	14
Caelo	Oxytetracycline hydrochloride	12130001	1
Gehe	Oxytetracycline hydrochloride	1205028-01	1
Euro OTC	Oxytetracycline hydrochloride	120502802	2
Fagron	Oxytetracycline hydrochloride	13D08-N11	6
Euro OTC	Oxytetracycline hydrochloride	12050-28	1
Euro OTC	Oxytetracycline hydrochloride	1306022-01	23
Caelo	Oxytetracycline hydrochloride	1306022-01	2
	Oxytetracycline hydrochloride		1
Phönix Gotha	Oxytetracycline hydrochloride	1232814	1
Caelo	Oxytetracycline hydrochloride	12328104	1
Caelo	Oxytetracycline hydrochloride	12328103	1
Anzag	Oxytetracycline hydrochloride	12328103	1
Caelo	Oxytetracycline hydrochloride	5041402	1
Caelo	Oxytetracycline hydrochloride	12328107	1
Euro OTC	Oxytetracycline hydrochloride	1306022	1
Fagron	Oxytetracycline hydrochloride	13L19-B33-290731	2
Fagron	Oxytetracycline hydrochloride	912A-02865	1
Fagron	Oxytetracycline hydrochloride	13L19-B33-290731	1
Euro OTC	Oxytetracycline hydrochloride	1205028	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	Oxytetracycline hydrochloride	13L19-B33	4
Caelo	Oxytetracycline hydrochloride	13L19-B33-290730	1
Fagron	Oxytetracycline hydrochloride	13I26-N11	1
Euro OTC	Oxytetracycline hydrochloride	130602201	1
Euro OTC	Oxytetracycline hydrochloride	1306022-02	13
	Oxytetracycline hydrochloride	130602202	1
Fagron	Oxytetracycline hydrochloride	13L19-B33-290730	3
Caelo	Oxytetracycline hydrochloride	13L19-B33	1
Caelo	Oxytetracycline hydrochloride	12091405	1
Euro OTC	Oxytetracycline hydrochloride	130602202	1
Bombastus	Oxytetracycline hydrochloride	13L19-B33-290732	1
	Oxytetracycline hydrochloride	1306022-02	3
Gehe	Oxytetracycline hydrochloride	1306022-02	1
Caelo	Oxytetracycline hydrochloride	14128003	1
Caelo	Oxytetracycline hydrochloride	1407012-01	1
Euro OTC	Oxytetracycline hydrochloride	1407012-01	14
Euro OTC	Oxytetracycline hydrochloride	28011505	1
	Oxytetracycline hydrochloride	140701201	1
Caelo	Oxytetracycline hydrochloride	14128004	1
Euro OTC	Oxytetracycline hydrochloride	1407012-02	13
Euro OTC	Oxytetracycline hydrochloride	1407011202	1
Phönix Gotha	Oxytetracycline hydrochloride	1407012-02	1
Fagron	Oxytetracycline hydrochloride	14/22-B01-301465	1
Fagron	Oxytetracycline hydrochloride	14122-B01-301463	1
Euro OTC	Oxytetracycline hydrochloride	15051507	1
Euro OTC	Oxytetracycline hydrochloride	1407012-03	5
Fagron	Oxytetracycline hydrochloride	1407012-01	1
Alliance	Oxytetracycline hydrochloride	1407012-03	1
Fagron	Oxytetracycline hydrochloride	4-49732A-2	1
Fagron	Oxytetracycline hydrochloride	14I22-B01-301465	1
Norbrook/Gehe	Oxytetracycline hydrochloride	140701203	1
Euro OTC	Oxytetracycline hydrochloride	1306022-03	5
Euro OTC	Oxytetracycline hydrochloride	140701203	1
Fagron	Oxytetracycline hydrochloride	14I22-B01-301464	1
Fagron	Oxytetracycline hydrochloride		1
Fagron	Oxytetracycline hydrochloride	130602203	1
Fagron	Oxytetracycline hydrochloride	14I22-B01	1
Fagron	Oxytetracycline hydrochloride	14/22-B01-301464	1
Euro OTC	Oxytetracycline hydrochloride	1506037-01	25
Caelo	Oxytetracycline hydrochloride	1506037-01	3
Caelo	Oxytetracycline hydrochloride	15060108	1
Euro OTC	Oxytetracycline hydrochloride	150603701	1
Norbrook Lab.Ltd.	Oxytetracycline hydrochloride	1506037-01	2
Caelo	Oxytetracycline hydrochloride	15060109	7
Noweda	Oxytetracycline hydrochloride	140701203	1
Noweda	Oxytetracycline hydrochloride	140701202	1
Laborchemie Apolda/Phönix	Oxytetracycline hydrochloride	1506037-02	1
Euro OTC	Oxytetracycline hydrochloride	1506037-02	27
Fagron	Oxytetracycline hydrochloride	15D29-B99-308608	1
Anzag	Oxytetracycline hydrochloride	1506037-02	1
Caelo	Oxytetracycline hydrochloride	1506037-02	1
Anzag	Oxytetracycline hydrochloride	1506037	1
Euro OTC	Oxytetracycline hydrochloride	15060109	2
Caesar&Loretz GmbH	Oxytetracycline hydrochloride	15060109	1
Euro OTC	Oxytetracycline hydrochloride	15060377-01	1
Caelo	Oxytetracycline hydrochloride	150603702	1
Euro OTC	Oxytetracycline hydrochloride	1506037	2
Euro OTC	Oxytetracycline hydrochloride	1506037-03	13
Fagro/Anzag	Oxytetracycline hydrochloride	14122-B01-301464	1
Caelo	Oxytetracycline hydrochloride	16077001	3

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Supplier	Substance	Batch	Spectra
Euro OTC	Oxytetracycline hydrochloride	1602025-01	16
Caelo	Oxytetracycline hydrochloride	16077003	3
Caelo	Oxytetracycline hydrochloride	16077008	4
Caelo	Oxytetracycline hydrochloride	16077002	2
Fagron	Oxytetracycline hydrochloride	15116-b02-322907	1
Caelo	Oxytetracycline hydrochloride	16044007	1
Fagron	Oxytetracycline hydrochloride	15L16-B02-322907	1
Caelo	Oxytetracycline hydrochloride	1506037	1
Fagron	Oxytetracycline hydrochloride	15L16-B02-322908	1
Caelo	Oxytetracycline hydrochloride	16077007	2
Euro OTC	Oxytetracycline hydrochloride	1602025-02	30
GEHE	Oxytetracycline hydrochloride	1602025-02	1
Euro OTC	Oxytetracycline hydrochloride	160202501	1
caesar	Oxytetracycline hydrochloride	16077008	2
Caelo	Oxytetracycline hydrochloride	16077011	1
Caelo	Oxytetracycline hydrochloride	16077009	1
Euro OTC	Oxytetracycline hydrochloride	1703130H/1602025-01	1
Euro OTC	Oxytetracycline hydrochloride	1602025	2
Caelo	Oxytetracycline hydrochloride	16077016	2
Apomix/Kehr	Oxytetracycline hydrochloride	16077014	1
Gehe	Oxytetracycline hydrochloride	1602025-02	2
Euro OTC	Oxytetracycline hydrochloride	1602025-1	1
Caelo	Oxytetracycline hydrochloride	16077012	1
Euro OTC	Oxytetracycline hydrochloride		1
Caelo	Oxytetracycline hydrochloride	16077017	1
Caelo	Oxytetracycline hydrochloride	1607716	1
Euro OTC	Oxytetracycline hydrochloride	1701034-01	16
Finteler Apotheke	Oxytetracycline hydrochloride	1602025-02	1
Caelo	Oxytetracycline hydrochloride	16340605	3
Apomix/Phoenix Leipzig ...	Oxytetracycline hydrochloride	1602025-02	1
Euro OTC	Oxytetracycline hydrochloride	160202502	1
GEHE	Oxytetracycline hydrochloride	1701034-01	1
Euro OTC	Oxytetracycline hydrochloride	YT160702059	1
Sanacorp	Oxytetracycline hydrochloride	1701034-01	1
Caelo	Oxytetracycline hydrochloride	16340610	7
Euro OTC	Oxytetracycline hydrochloride	170034-01	1
Caelo	Oxytetracycline hydrochloride	16340606	3
Euro OTC	Oxytetracycline hydrochloride	1701034-015415	1
Caelo	Oxytetracycline hydrochloride	1701034-01	1
Caelo	Oxytetracycline hydrochloride	1/01034-02	1
Caelo	Oxytetracycline hydrochloride	1701034-02	1
Euro OTC	Oxytetracycline hydrochloride	1701034-02	17
Euro OTC	Oxytetracycline hydrochloride	1407012-09	1
Caelo	Oxytetracycline hydrochloride	16340611	1
Euro OTC	Oxytetracycline hydrochloride	1801033-01	6
Caelo	Oxytetracycline hydrochloride	17316806	2
Caelo	Oxytetracycline hydrochloride	163406010	1
Caelo	Oxytetracycline hydrochloride	17316805	1
Caelo	Oxytetracycline hydrochloride	17316812	1
Euro OTC	Oxytetracycline hydrochloride	1801033	1
Gehe	Oxytetracycline hydrochloride	17316805	1
Euro OTC	Oxytetracycline hydrochloride	21111815	1
Euro OTC	Oxytetracycline hydrochloride	1801033-02	2
Fagron	Oxytetracycline hydrochloride	1801033-01	1

- 78 481 spectra from 565 *Apo-Ident* customers from a total of 26 029 batches from a further 693 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 *Oxytetracycline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxytetracycline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	580	0	73 916
Type B	0	300	0	126 592
Type C	0	440	8	78 481

The substance/substance group *Oxytetracycline hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.9655 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.8817 %)	98.2143 % (> 97.5446 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21039	21600	8.65	44.96
21600	21600	0.00	45.15
21836	21836	0.00	32.50
21915	22503	13.77	39.20
22839	22669	9.34	27.11
23137	23137	0.00	35.73
23970	23137	7.38	37.17
22658	22658	0.00	33.64
22669	22669	0.00	33.89
20847	21999	8.86	32.97
21999	21999	0.00	38.04
22503	22503	0.00	34.57
22546	22546	0.00	37.10
20848	22503	7.56	30.56

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Pancreas powder**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20976-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Pancreas powder; Pancreatis pulvis

Special notes

When selecting the *Pancreas powder* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Pancreas powder*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pancreas powder	13118902	20976	40	1402190
Caelo	Pancreas powder	13395203	21481	40	20131218
Caelo	Pancreas powder	161397	22482	40	20160527*

Validation samples

A total of 280 317 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 *Pancreas powder*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Pancreas powder*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pancreas powder	13395203	21481 [†]	20
Caelo	Pancreas powder	161397	22482 [†]	20
Caelo	Pancreas powder	16139708	23757	40
Caelo	Pancreas powder	16139708	23758	40
Caelo	Pancreas powder	173226	23797	40

- 126 732 spectra from a total of 2785 batches from further 781 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 *Pancreas powder*.

*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*.

- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Pancreas powder* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pancreas powder* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	0	126 732
Type C	0	0	0	78 929

The substance/substance group *Pancreas powder* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	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
22482	22482	0.00	45.13
20976	20976	0.00	41.16
21481	22482	12.02	40.47

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Papaverine hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20481-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Papaverine hydrochloride; Papaverini hydrochloridum

Special notes

When selecting the *Papaverine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Papaverine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Papaverine hydro...	13324310	21735	40	20130920
Caelo	Papaverine hydro...	123161	23054	40	20121127*

Validation samples

A total of 280 317 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 *Papaverine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Papaverine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Papaverine hydrochloride	13324310	21735 [†]	20
Caelo	Papaverine hydrochloride	163159	23053	40
Caelo	Papaverine hydrochloride	16315911	23928	40

- 126 792 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 11 spectra from 8 *Apo-Ident* customers from 10 batches from the substance/substance group *Papaverine hydrochloride*.

*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	Papaverine hydrochloride		1
Phönix Gotha	Papaverine hydrochloride	12166101	1
Caelo	Papaverine hydrochloride	12166112	1
Caelo	Papaverine hydrochloride	12316105	1
GATT-KOLLER/PHOENIX	Papaverine hydrochloride	2927/07131314	1
Caelo	Papaverine hydrochloride	12166105	1
Caelo	Papaverine hydrochloride	13324307	1
Phönix Gotha	Papaverine hydrochloride	13324306	1
Caelo	Papaverine hydrochloride	15160608	2
Caelo	Papaverine hydrochloride	16315903	1

- 78 918 spectra from 565 *Apo-Ident* customers from a total of 26 127 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Papaverine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Papaverine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	100	0	126 792
Type C	0	10	1	78 918

The substance/substance group *Papaverine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8818 %)	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
21735	23054	13.51	69.46
23054	23054	0.00	61.87

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Paracetamol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20972-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Paracetamol; Paracetamolum

Special notes

When selecting the *Paracetamol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Paracetamol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Paracetamol	13D30-N03	20972	40	1402271
Fagron	Paracetamol	13D16-N08	20973	40	1402296
Fagron	Paracetamol	13G23-N03	20974	40	1402297
Euro OTC	Paracetamol	1111024-02	21598	40	20120123
Caelo	Paracetamol	15075706	22608	40	20150424

Validation samples

A total of 280317 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 *Paracetamol*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 *Paracetamol*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Paracetamol	1111024-02	21598 [†]	20
Caelo	Paracetamol	15075707	22822	40
Caelo	Paracetamol	170284	23852	40
Caelo	Paracetamol	180830	24053	40

- 126752 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 26 spectra from 13 *Apo-Ident* customers from 21 batches from the substance/substance group *Paracetamol*.

[†]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	Paracetamol	1111024-01	1
Caelo	Paracetamol	11300108	1
Caelo	Paracetamol	10065102	1
Euro OTC	Paracetamol	1111024-02	1
Caelo	Paracetamol	11300120	2
Caelo	Paracetamol	10325020	1
Caelo	Paracetamol	1912M-02045	1
Caelo	Paracetamol	13082011	1
Caelo	Paracetamol	13082010	2
Caelo	Paracetamol	1814U-02045	1
Caelo	Paracetamol	15075704	4
Caelo	Paracetamol	13082005	1
Caelo	Paracetamol	15245902	1
Caelo	Paracetamol	2815I-02045	1
Caelo	Paracetamol	15217704	1
Jenne	Paracetamol	15245901	1
Caelo	Paracetamol	15217708	1
Caelo	Paracetamol	15217712	1
Caelo	Paracetamol	15075708	1
Caelo	Paracetamol	15217710	1
Euro OTC	Paracetamol	17028409	1

- 78 903 spectra from 565 *Apo-Ident* customers from a total of 26 116 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Paracetamol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Paracetamol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	140	0	126 752
Type C	0	24	2	78 903

The substance/substance group *Paracetamol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.8817 %)	92.3077 % (> 80.7692 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22608	20972	9.57	42.59
20972	20972	0.00	46.09
20973	20973	0.00	49.52
21598	20972	2.35	51.16
20974	20974	0.00	36.88

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Patent blue V
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20469-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Patent blue V

Special notes

When selecting the *Patent blue V* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Patent blue V*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Patent blue V	12364206	21384	40	1508043
Caelo	Patent blue V	12364206	21385	40	20130110
Caelo	Patent blue V	13351803	21695	40	20131114
Caelo	Patent blue V	13351807	22387	40	1702362

Validation samples

A total of 280317 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 *Patent blue V*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1620 batches from further 372 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 *Patent blue V*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Patent blue V	13351803	21695 [†]	20
Caelo	Patent blue V	16306902	23214	40
Caelo	Patent blue V	16306902	23215	40

- 126792 spectra from a total of 2787 batches from further 781 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 18 *Apo-Ident* customers from 9 batches from the substance/substance group *Patent blue V*.

[†]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	Patent blue V	11305302	1
Caelo	Patent blue V	11305303	3
Caelo	Patent blue V	12364202	1
Caelo	Patent blue V	12364206	2
Caelo	Patent blue V	13351803	1
Caelo	Patent blue V	13351807	5
Caelo	Patent blue V	15060204	1
Caelo	Patent blue V	13351808	1
Caelo	Patent blue V	17034204	3
Bombastus	Patent blue V	17034204	1

- 78 910 spectra from 565 *Apo-Ident* customers from a total of 26 128 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Patent blue V* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Patent blue V* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	27	73	126 792
Type C	0	13	6	78 910

The substance/substance group *Patent blue V* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	27.0000 % (> 24.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
21384	21384	0.00	111.86
21385	21384	1.81	111.81
21695	22387	3.22	113.27
22387	22387	0.00	112.86

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Phenazone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22532-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Phenazone; Phenazonum

Special notes

When selecting the *Phenazone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Phenazone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Phenazone	13G16-B07-287172	22532	40	AR-16-FG-011360-01
Caelo	Phenazone	15415107	22827	40	20151215
Caelo	Phenazone	181347	24259	40	20180629*

Validation samples

A total of 280 317 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 *Phenazone*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Phenazone*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Phenazone	15415101	22576	40
Fagron	Phenazone	13G16-B07-287172	22720	40
Caelo	Phenazone	170836	23302	40
Caelo	Phenazone	182565	24369	40

- 126 732 spectra from a total of 2785 batches from further 781 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 *Phenazone*.

*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
Caelo	Phenazone	18061101	1

- 78 928 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Phenazone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Phenazone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	0	126 732
Type C	0	1	0	78 928

The substance/substance group *Phenazone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8830 %)	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
22532	22532	0.00	31.83
22827	24259	6.25	28.91
24259	24259	0.00	29.68

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Pheniramine maleate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20694-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Pheniramine maleate; Pheniramine maleas

Special notes

When selecting the *Pheniramine maleate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Pheniramine maleate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pheniramine male...	12200502	20694	40	1401559
Euro OTC	Pheniramine male...	1109013-02	20756	40	20111122
Fagron	Pheniramine male...	13D24-N04	20928	40	20130530

Validation samples

A total of 280317 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 *Pheniramine maleate*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 *Pheniramine maleate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pheniramine maleate	15172702	22790	40
Euro OTC	Pheniramine maleate	1701021	23384	40
Caelo	Pheniramine maleate	173167	23821	40

- 126772 spectra from a total of 2786 batches from further 781 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 26 *Apo-Ident* customers from 26 batches from the substance/substance group *Pheniramine maleate*.

Supplier	Substance	Batch	Spectra
Fagron	Pheniramine maleate	12I06-N02	1
Fagron	Pheniramine maleate	12L04-N05	3
Caelo	Pheniramine maleate	9276210	1
Alliance Healthcare	Pheniramine maleate	12L04-N05	1
Caelo	Pheniramine maleate	12352604	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Pheniramine maleate	1209032-01	2
Cealo	Pheniramine maleate	12352608	1
Caelo	Pheniramine maleate	14C25-B01-292540	1
Caelo	Pheniramine maleate	12352602	1
Fagron	Pheniramine maleate	14C25-B01-29540	1
Fagron	Pheniramine maleate	14C25-B01-295293	3
Supriya LifeScience Ltd...	Pheniramine maleate	14C25-B01	1
Euro OTC	Pheniramine maleate	1411044-01	1
Caelo	Pheniramine maleate	14C25-B01-302272	1
Fagron	Pheniramine maleate	14C25-B01-307150	2
Caelo	Pheniramine maleate	1235611	1
Supriya LifeScience Ltd...	Pheniramine maleate	SLL/P/1213063	1
Euro OTC	Pheniramine maleate	1411044-02	2
Caelo	Pheniramine maleate	15172704	1
Fagron	Pheniramine maleate	14c25-b01-307150	1
Fagron	Pheniramine maleate	14c25b01307150	1
Caelo	Pheniramine maleate	15172711	1
Caelo	Pheniramine maleate	14C25-B01-322989	1
Fagron	Pheniramine maleate	14C25-B01-328732	2
Euro OTC	Pheniramine maleate	1701021-01	4
Caelo	Pheniramine maleate	17316702	1
Caelo	Pheniramine maleate	15172708	1

- 78 891 spectra from 565 *Apo-Ident* customers from a total of 26 111 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Pheniramine maleate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pheniramine maleate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	120	0	126 772
Type C	0	29	9	78 891

The substance/substance group *Pheniramine maleate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	76.3158 % (> 68.4211 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20694	20694	0.00	54.46
20756	20694	18.27	56.40
20928	20694	8.18	54.47

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Phenylbutazon**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20447-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Phenylbutazon; Phenylbutazonum

Special notes

When selecting the *Phenylbutazon* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Phenylbutazon*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Phenylbutazon	14057202	21379	40	20140321
Euro OTC	Phenylbutazon	1305050-02	21605	40	AR-15-FG-005687-01
Euro OTC	Phenylbutazon	1507023	21855	40	20150805*

Validation samples

A total of 280 317 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 *Phenylbutazon*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Phenylbutazon*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Phenylbutazon	1305050-02	21605 [†]	20
Euro OTC	Phenylbutazon	1507023	21855 [†]	20
Caelo	Phenylbutazon	161121	22471	60
Euro OTC	Phenylbutazon	1604033	22563	40
Euro OTC	Phenylbutazon	1804018	24122	40

- 126 712 spectra from a total of 2784 batches from further 781 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 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Phenylbutazon*.

*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	Phenylbutazon	10262901	1
Fagron	Phenylbutazon	11H26-N02	1
Caelo	Phenylbutazon	15218502	1
Euro OTC	Phenylbutazon	19091806	1
Euro OTC	Phenylbutazon	170612PB/1604033-01	1

- 78 924 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Phenylbutazon* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Phenylbutazon* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	180	0	126 712
Type C	0	5	0	78 924

The substance/substance group *Phenylbutazon* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8819 %)	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
21379	21855	4.47	34.86
21605	21605	0.00	36.89
21855	21855	0.00	32.22

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Phenylephrine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20567-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Phenylephrine hydrochloride; Phenylephrini hydrochloridum

Special notes

When selecting the *Phenylephrine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Phenylephrine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Phenylephrine hy...	12J19-B40-288254	21051	40	20131210
Fagron	Phenylephrine hy...	14H13-B02-308438	21960	40	AR-16-FG-008920-01
Fagron	Phenylephrine hy...	16A20-B07-317987	22388	40	AR-16-FG-013385-01
Euro OTC	Phenylephrine hy...	1704009	23394	40	20170524*

Validation samples

A total of 280 317 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 *Phenylephrine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Phenylephrine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Phenylephrine hydrochloride	14H13-B02-308438	21960 [†]	20
Fagron	Phenylephrine hydrochloride	17C23-B04-333878	23263	40
Fagron	Phenylephrine hydrochloride	17C23-B04-333880	23267	40

- 126 792 spectra from a total of 2786 batches from further 781 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*.

- 49 spectra from 12 *Apo-Ident* customers from 31 batches from the substance/substance group *Phenylephrine hydrochloride*.

Supplier	Substance	Batch	Spectra
Noweda	Phenylephrine hydrochloride	12F01-N20	2
Fagron	Phenylephrine hydrochloride	12C08-N17	1
Fagron	Phenylephrine hydrochloride	12A03-N09	1
Fagron	Phenylephrine hydrochloride	12g19-n04	1
Fagron	Phenylephrine hydrochloride	13A03-N09	3
Fagron	Phenylephrine hydrochloride	12G19-N04	1
Fagron	Phenylephrine hydrochloride	12J19-B40-288253	2
Fagron	Phenylephrine hydrochloride	13G10-N04	1
Fagron	Phenylephrine hydrochloride	13B14-N03	1
Fagron	Phenylephrine hydrochloride	1021402	1
Fagron/Sanacorp	Phenylephrine hydrochloride	13K25-B02-293844	3
Fagron	Phenylephrine hydrochloride	14H13B02-299817	1
Fagron	Phenylephrine hydrochloride	14H13B02299817	1
Fagron	Phenylephrine hydrochloride	10091504	1
Fagron	Phenylephrine hydrochloride	14H13-B02-299816	2
Fagron	Phenylephrine hydrochloride	13K25-B02-293845	1
Fagron	Phenylephrine hydrochloride	14H13-B02-309892	3
Fagron	Phenylephrine hydrochloride	15F09-B08-316796	1
Jenne	Phenylephrine hydrochloride	14H13-B02	2
Fagron	Phenylephrine hydrochloride	14H13-B02-299814	1
Caelo	Phenylephrine hydrochloride	14H13-B02-308438	1
Fagron	Phenylephrine hydrochloride	16A20-B07-317987	2
Phoenix	Phenylephrine hydrochloride	15F09-B08	1
ALH	Phenylephrine hydrochloride	16A20-B07-322159	1
Fagron	Phenylephrine hydrochloride	16A20-B07-323398	3
Fagron	Phenylephrine hydrochloride	17C23-B04-333878	1
Fagron	Phenylephrine hydrochloride	17C23-B04-333880	1
Fagron	Phenylephrine hydrochloride	17C23-B04-334819	3
Fagron	Phenylephrine hydrochloride	17c23-b04-333880	1
Noweda	Phenylephrine hydrochloride	17C23-B04-336301	4
Fagron	Phenylephrine hydrochloride	12031801	1

- 78 880 spectra from 565 *Apo-Ident* customers from a total of 26 107 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Phenylephrine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Phenylephrine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	100	0	126 792
Type C	0	45	4	78 880

The substance/substance group *Phenylephrine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	91.8367 % (> 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
21051	21960	2.41	40.38
21960	21960	0.00	40.80
23394	23394	0.00	41.95
22388	22388	0.00	41.12

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Phenytoin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20949-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Phenytoin; Phenytoinum

Special notes

When selecting the *Phenytoin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Phenytoin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Phenytoin	13G26-N02	20949	40	1401380
Fagron	Phenytoin	15E12-B05-312661	22271	30	20150519
Fagron	Phenytoin	18F01-B02-350492	24438	40	20180705

Validation samples

A total of 280 317 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 *Phenytoin*. These samples are listed above in the [calibration samples](#) section.
- 74 386 spectra from a total of 1620 batches from further 372 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 [†].

- 175 spectra of 5 reference samples from the substance/substance group *Phenytoin*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Phenytoin	12I07-N02	20678	40
Fagron	Phenytoin	15E12-B05-312661	22271 [†]	15
Fagron	Phenytoin	16C14-B06-325086	23110	40
Fagron	Phenytoin	16C14-B06-325086	23377	40
Fagron	Phenytoin	17L22-B04-345861	23994	40

- 126 717 spectra from a total of 2785 batches from further 781 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 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Phenytoin*.

[†]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
Fagron	Phenytoin	12C27N13	1
Fagron	Phenytoin	12I07-N02	1
Fagron	Phenytoin	13G26-N02	1

- 78 926 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Phenytoin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Phenytoin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 386
Type B	0	175	0	126 717
Type C	0	2	1	78 926

The substance/substance group *Phenytoin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 94.5455 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.5714 %)
Type C	100.0000 % (> 99.8821 %)	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
20949	20949	0.00	94.97
22271	20949	10.04	95.46
24438	20949	4.34	95.24

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Pilocarpine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21519-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Pilocarpine hydrochloride; Pilocarpini hydrochloridum

Special notes

When selecting the *Pilocarpine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Pilocarpine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pilocarpine hydr...	12217319	21519	40	1501660
Euro OTC	Pilocarpine hydr...	1305044-01	21629	40	20130725
Euro OTC	Pilocarpine hydr...	1603047	22553	40	20160429*
Caelo	Pilocarpine hydr...	17124208	23371	40	20170607
Euro OTC	Pilocarpine hydr...	1305044-01	21629SI	40	20130725
Euro OTC	Pilocarpine hydr...	1603047	22553SI	40	20160429*

Validation samples

A total of 280 317 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 *Pilocarpine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1619 batches from further 372 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 [†].

- 460 spectra of 12 reference samples from the substance/substance group *Pilocarpine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pilocarpine hydrochloride	12217319	21518	60
Caelo	Pilocarpine hydrochloride	12217319	21519 [†]	20
Euro OTC	Pilocarpine hydrochloride	1305044-01	21629 [†]	20
Caelo	Pilocarpine hydrochloride	171595	23337	40
Caelo	Pilocarpine hydrochloride	171242	23338	40
Euro OTC	Pilocarpine hydrochloride	1806012	24140	40
Caelo	Pilocarpine hydrochloride	12217319	21518SI	60
Euro OTC	Pilocarpine hydrochloride	1305044-01	21629SI [†]	20
Caelo	Pilocarpine hydrochloride	171595	23337SI	40
Caelo	Pilocarpine hydrochloride	171242	23338SI	40
Caelo	Pilocarpine hydrochloride	17124208	23371SI	40
Euro OTC	Pilocarpine hydrochloride	1806012	24140SI	40

- 126 432 spectra from a total of 2783 batches from further 781 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.

- 45 spectra from 37 *Apo-Ident* customers from 22 batches from the substance/substance group *Pilocarpine hydrochloride*.

Supplier	Substance	Batch	Spectra
Euro OTC	Pilocarpine hydrochloride	Euroo	1
Caelo	Pilocarpine hydrochloride	2211112032607	1
Euro OTC	Pilocarpine hydrochloride	1202031-01	1
Caelo	Pilocarpine hydrochloride	25051303	1
Caelo	Pilocarpine hydrochloride	12K07-N09	1
Caelo	Pilocarpine hydrochloride	12217302	1
Euro OTC	Pilocarpine hydrochloride	1202031-02	1
Caelo	Pilocarpine hydrochloride	12217307	1
Euro OTC	Pilocarpine hydrochloride	1305044-01	5
Sanacorp	Pilocarpine hydrochloride	12217302	1
Caelo	Pilocarpine hydrochloride	12217316	1
Euro OTC	Pilocarpine hydrochloride	130504401	2
Fagron	Pilocarpine hydrochloride	13H24-N03	1
Euro OTG	Pilocarpine hydrochloride	1305044-01	1
Euro OTC	Pilocarpine hydrochloride	13050-14-01	1
Caelo	Pilocarpine hydrochloride	130504401	1
Euro OTC	Pilocarpine hydrochloride	1305044-03	2
Caelo	Pilocarpine hydrochloride	1305044-03	1
Euro OTC	Pilocarpine hydrochloride	1603047-01	2
Gehe	Pilocarpine hydrochloride	15198610	1
Caelo	Pilocarpine hydrochloride	17124208	3
Euro OTC	Pilocarpine hydrochloride	1603047	1
Caelo	Pilocarpine hydrochloride	17236401	1
Euro OTC	Pilocarpine hydrochloride	1603047-02	9
Caelo	Pilocarpine hydrochloride	1603047-02	2
Caelo	Pilocarpine hydrochloride	18138704	1
Euro OTC	Pilocarpine hydrochloride	1806012-01	1

- 78 884 spectra from 565 *Apo-Ident* customers from a total of 26 115 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Pilocarpine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pilocarpine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	454	6	126 432
Type C	0	39	6	78 884

The substance/substance group *Pilocarpine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	98.6957 % (> 98.0435 %)
Type C	100.0000 % (> 99.8817 %)	86.6667 % (> 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
23371	21519	6.39	34.85
21519	21519	0.00	32.21
21629	22553	4.73	34.63
22553	22553	0.00	32.77

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Poloxamers 407**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20540-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Poloxamers 407; Poloxamera

Special notes

When selecting the *Poloxamers 407* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Poloxamers 407*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Poloxamers 407	14196101	21652	40	AR-14-FG-013090-01
Fagron	Poloxamers 407	14G17-B03-296866	21726	40	20140806
Caelo	Poloxamers 407	16242605	23257	40	20160915

Validation samples

A total of 280317 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 *Poloxamers 407*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 *Poloxamers 407*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Poloxamers 407	14196101	21652 [†]	20
Fagron	Poloxamers 407	14G17-B03-296866	21726 [†]	20
Caelo	Poloxamers 407	170486	23311	40
Caelo	Poloxamers 407	172921	23810	40
Caelo	Poloxamers 407	181607	24219	40
Caelo	Poloxamers 407	182636	24358	40

- 126692 spectra from a total of 2783 batches from further 781 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.

- 53 spectra from 33 *Apo-Ident* customers from 31 batches from the substance/substance group *Poloxamers 407*.

[†]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
Phonix	Poloxamers 407	12/13-N10	1
Caelo	Poloxamers 407	12286801	2
Caelo	Poloxamers 407	12286805	1
Fagron	Poloxamers 407	12K23-N03	1
Caelo	Poloxamers 407	13133201	1
Fagron	Poloxamers 407	13G29-N01	1
Caelo	Poloxamers 407	12286806	1
Fagron	Poloxamers 407	WPWI610C	1
Fagron	Poloxamers 407	13G29-N01	1
Caelo	Poloxamers 407	13133203	2
Fagron	Poloxamers 407	5211Q-07027	1
Caelo	Poloxamers 407	13133207	1
Caelo	Poloxamers 407	14196101	2
Fagron	Poloxamers 407	914I-07027	1
Caelo	Poloxamers 407	14196108	2
Caelo	Poloxamers 407	14359501	1
Sanacorp	Poloxamers 407	14196101	2
Caelo	Poloxamers 407	14196105	1
Fagron	Poloxamers 407	15A26-B03-303503	1
Fagron	Poloxamers 407	315E-07027	1
Caelo	Poloxamers 407	14196104	1
Caesar & Loretz GmbH	Poloxamers 407	15183102	1
Caelo	Poloxamers 407	15397802	5
Caelo	Poloxamers 407	16189302	4
Caelo	Poloxamers 407	15183102	2
Fagron	Poloxamers 407	5315I-07027	1
Caelo	Poloxamers 407	16242601	3
Caelo	Poloxamers 407	16189301	1
Caelo	Poloxamers 407	162426056	1
Caelo	Poloxamers 407	17048601	1
Caelo	Poloxamers 407	16242605	1
Caelo	Poloxamers 407	17292101	2
Caelo	Poloxamers 407	18025101	5

- 78 876 spectra from 565 *Apo-Ident* customers from a total of 26 106 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Poloxamers 407* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Poloxamers 407* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	200	0	126 692
Type C	0	49	4	78 876

The substance/substance group *Poloxamers 407* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8817 %)	92.4528 % (> 86.7925 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21652	21652	0.00	44.51
21726	21652	4.21	44.47
23257	21652	3.00	44.34

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Polymyxin B sulfate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20853-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Polymyxin B sulfate; Polymyxin B sulphate; Polymyxini B sulfas

Special notes

When selecting the *Polymyxin B sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Polymyxin B sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Polymyxin B sulf...	13C12-N02	20853	40	1402691
Euro OTC	Polymyxin B sulf...	1304033-01	21094	39	20130829
Fagron	Polymyxin B sulf...	12G13-N05	21258	40	1410347
Euro OTC	Polymyxin B sulf...	1202039-02	21329	40	1411033
Euro OTC	Polymyxin B sulf...	1304033-02	21584	40	20130612

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Polymyxin B sulf. ...	13I13-N05	21595	30	AR-15-FG-001516-01
Fagron	Polymyxin B sulf. ...	14F04-B03-296722	21957	40	20140708
Euro OTC	Polymyxin B sulf. ...	1505005-01	21980	40	AR-16-FG-005387-01
Fagron	Polymyxin B sulf. ...	15H14-B01-314364	22323	40	20150902
Caelo	Polymyxin B sulf. ...	153501	22451	40	20160318*
Euro OTC	Polymyxin B sulf. ...	1604016	22542	40	20160509*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 429 spectra of 11 reference samples from the substance/substance group *Polymyxin B sulfate*. These samples are listed above in the [calibration samples](#) section.
- 74 067 spectra from a total of 1612 batches from further 372 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 [†].

- 396 spectra of 14 reference samples from the substance/substance group *Polymyxin B sulfate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Polymyxin B sulfate	1202039-02	20904	40
Fagron	Polymyxin B sulfate	13E06-N12	20912	40
Euro OTC	Polymyxin B sulfate	1304033-01	21094 [†]	1
Euro OTC	Polymyxin B sulfate	1304033-02	21584 [†]	20
Fagron	Polymyxin B sulfate	13I13-N05	21595 [†]	15
Fagron	Polymyxin B sulfate	14F04-B03-296722	21957 [†]	20
Euro OTC	Polymyxin B sulfate	1505005-01	21980 [†]	20
Fagron	Polymyxin B sulfate	15H14-B01-314364	22323 [†]	20
Caelo	Polymyxin B sulfate	153501	22451 [†]	20
Euro OTC	Polymyxin B sulfate	1701010	23012	40
Euro OTC	Polymyxin B sulfate	1707013	23554	40
Euro OTC	Polymyxin B sulfate	1802006	23953	40
Euro OTC	Polymyxin B sulfate	1807004	24143	40
Caelo	Polymyxin B sulfate	181154	24407	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.

- 126 496 spectra from a total of 2775 batches from further 781 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.

- 72 spectra from 56 *Apo-Ident* customers from 37 batches from the substance/substance group *Polymyxin B sulfate*.

Supplier	Substance	Batch	Spectra
Fagron	Polymyxin B sulfate	12D05-N01	1
Euro OTC	Polymyxin B sulfate	25101201	1
Euro OTC	Polymyxin B sulfate	1202039-01	1
Phönix	Polymyxin B sulfate	1202039-01	1
EuRho	Polymyxin B sulfate	1202039-01	1
Alliance Healthcare	Polymyxin B sulfate	1202039-02	1
Euro OTC	Polymyxin B sulfate	1202039-02	4
Fagron	Polymyxin B sulfate	13G05-N06	2
Euro OTC	Polymyxin B sulfate	1304033-01	1
Euro OTC	Polymyxin B sulfate	1304033-02	1
Euroo/Phoenix	Polymyxin B sulfate	1304033-02	1
Euro OTC	Polymyxin B sulfate	11091419	1
Caelo	Polymyxin B sulfate	13H28-B02-287953	1
Euro OTC	Polymyxin B sulfate	1406012-01	3
Fagron	Polymyxin B sulfate	13/13-N05	1
Fagron	Polymyxin B sulfate	12G13-N05	1
Fagron	Polymyxin B sulfate	13H28-B02-287954	1
Fagron	Polymyxin B sulfate	14F04-B03-296721	1
Euro OTC	Polymyxin B sulfate	140601202	2
Euro OTC	Polymyxin B sulfate	1406012-02	4
Euro OTC	Polymyxin B sulfate	23051502	1
Caelo	Polymyxin B sulfate	1102013-01	1
Euro OTC	Polymyxin B sulfate	1304033-03	1
Euro OTC	Polymyxin B sulfate	1505005-01	4
Euro OTC	Polymyxin B sulfate	150500501	1
Rondell Apotheke	Polymyxin B sulfate	121161	1
Caelo	Polymyxin B sulfate	1604016-01	3
Fagron	Polymyxin B sulfate	912A-03315	1
Bombastus	Polymyxin B sulfate	1604016-02	1
Euro OTC	Polymyxin B sulfate	1604016-02	1
Fagron	Polymyxin B sulfate	15H14-B01-315692	1
Euro OTC	Polymyxin B sulfate	1701010-01	4
Fagron	Polymyxin B sulfate	16C01-B04-322012	2
Euro OTC	Polymyxin B sulfate	28041730	1
Fagron	Polymyxin B sulfate	16C01-B04	1
Caelo	Polymyxin B sulfate	1701010-01	1
Gehe	Polymyxin B sulfate	170101001	1
GEHE	Polymyxin B sulfate	1701010-01	1
Caelo	Polymyxin B sulfate	170101001	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	Polymyxin B sulfate	1701010-01	1
Caelo	Polymyxin B sulfate	150725	1
Sanacorp	Polymyxin B sulfate	1707013-01	1
cealo	Polymyxin B sulfate	16c01-b04-319432	1
Euro OTC	Polymyxin B sulfate	1707013-01	3
Caelo	Polymyxin B sulfate	1707013-01	1
Caelo	Polymyxin B sulfate	1802006-011	1
Euro OTC	Polymyxin B sulfate	1802006-01	2
Fagron	Polymyxin B sulfate	16G21-B03-333808	1
Euro OTC	Polymyxin B sulfate	170101001	1
Caelo	Polymyxin B sulfate	1802006-01	1

- 78 857 spectra from 565 *Apo-Ident* customers from a total of 26 101 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Polymyxin B sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Polymyxin B sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	428	1	74 067
Type B	0	370	26	126 496
Type C	0	66	6	78 857

The substance/substance group *Polymyxin B sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	99.7669 % (> 99.0676 %)
Type B	100.0000 % (> 99.9901 %)	93.4343 % (> 92.6768 %)
Type C	100.0000 % (> 99.8817 %)	91.6667 % (> 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
21329	21329	0.00	26.20
21595	21595	0.00	21.30
20853	20853	0.00	17.31
21957	22451	1.45	30.75
21258	21258	0.00	14.93
22542	22542	0.00	17.92
21094	21980	2.97	21.08
21584	21980	2.99	19.73
21980	21980	0.00	23.68
22323	21258	5.65	20.49
22451	22451	0.00	30.49

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Potassium citrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20021-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Potassium citrate; Kalii citras

Special notes

When selecting the *Potassium citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Potassium citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potassium citrate	11320212	20655	40	20111201
Caelo	Potassium citrate	13317618	21452	40	20130926
Caelo	Potassium citrate	15123103	21775	40	20150414
Euro OTC	Potassium citrate	1509044	21936	40	20151013*
Caelo	Potassium citrate	161130	22476	40	20160602*
Euro OTC	Potassium citrate	1611017	22921	40	20161207*

Validation samples

A total of 280317 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 *Potassium citrate*. These samples are listed above in the [calibration samples](#) section.
- 74256 spectra from a total of 1617 batches from further 372 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 11 reference samples from the substance/substance group *Potassium citrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Potassium citrate	13317618	21452 [†]	20
Caelo	Potassium citrate	15123103	21775 [†]	20
Euro OTC	Potassium citrate	1509044	21936 [†]	20
Caelo	Potassium citrate	161130	22476 [†]	20
Euro OTC	Potassium citrate	1603040	22521	40
Euro OTC	Potassium citrate	1606041	22676	40
Caelo	Potassium citrate	170929	23290	40
Euro OTC	Potassium citrate	1705024	23428	40
Caelo	Potassium citrate	180385	24046	40
Euro OTC	Potassium citrate	1803003	24084	40
Euro OTC	Potassium citrate	1807034	24160	40

- 126532 spectra from a total of 2778 batches from further 781 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.

- 233 spectra from 111 *Apo-Ident* customers from 100 batches from the substance/substance group *Potassium citrate*.

Supplier	Substance	Batch	Spectra
Caelo	Potassium citrate	1234	4
Caelo	Potassium citrate	11320201	1
Caelo	Potassium citrate	3456	1
Caelo	Potassium citrate		8
Caelo	Potassium citrate	5555	1
Caelo	Potassium citrate	11320212	3
Caelo	Potassium citrate	1112008-01	1
Caelo	Potassium citrate	12135302	6
lohmann	Potassium citrate	1051470	1
Caelo	Potassium citrate	11102201	1
Caelo	Potassium citrate	12135303	2
Sanacorp/ euRho	Potassium citrate	1204016-01	1
Sanacorb	Potassium citrate	12135311	2
Caelo	Potassium citrate	9259107	1
Caelo	Potassium citrate	12135309	2
Caelo	Potassium citrate	1215309	1
Caelo	Potassium citrate	12299201	5
Hiperscan	Potassium citrate		1
Caelo	Potassium citrate	1204016-01	1
Caelo	Potassium citrate	12299203	4
Caelo	Potassium citrate	12135311	1
Fagron	Potassium citrate	1234567	1
Caelo	Potassium citrate	71730128	1
Caelo	Potassium citrate	13080602	8
Phönix	Potassium citrate	1211006-01	2
Caelo	Potassium citrate	12299202	1
Caelo	Potassium citrate	9259120	1
Euro OTC	Potassium citrate	22101303	1
HiperScan	Potassium citrate		1
Caelo	Potassium citrate	13080603	1
Fagron	Potassium citrate		1
Caelo	Potassium citrate	13135904	1
ghfgh	Potassium citrate	3654645	1
Euro OTC	Potassium citrate	1311036-01	9
Caelo	Potassium citrate	411025-1-P	1
Labor	Potassium citrate	1234	2
Euro OTC	Potassium citrate	1306032-01	1
Caelo	Potassium citrate	71730367	1
Caelo	Potassium citrate	13317603	2
Caelo	Potassium citrate	13317604	2
Caelo	Potassium citrate	28021402	1
Caelo	Potassium citrate	13135902	1
Caelo	Potassium citrate	3112M01737	1
Caelo	Potassium citrate	13135907	3
Caelo	Potassium citrate	13135908	1
Caelo	Potassium citrate	13317602	2
Caelo	Potassium citrate	123Testmessung	1
Caelo	Potassium citrate	12334	1
Caelo	Potassium citrate	123Test	3
Caelo	Potassium citrate	13317613	2
EuRho/Phönix	Potassium citrate	1311036-01	1
Caelo	Potassium citrate	2114M1737	1

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Supplier	Substance	Batch	Spectra
Caelo	Potassium citrate	17061402	1
Testsubstanz	Potassium citrate		1
Gutenberg-Apotheke	Potassium citrate	13135907	1
Phoenix 08.07.2014	Potassium citrate	13317624	1
Phoenix	Potassium citrate	1326PLV-1739	1
Caelo	Potassium citrate	123test	2
Euro OTC	Potassium citrate	1406025-01	1
Caelo	Potassium citrate	13317618	2
Caelo	Potassium citrate	14138107	1
Caelo	Potassium citrate	5021509	1
Phoenix Goettin	Potassium citrate	13317613	1
Euro OTC	Potassium citrate	1410014-01	2
Caelo	Potassium citrate	14138105	6
Caelo	Potassium citrate	14138119	1
Caelo	Potassium citrate	14138118	2
Caelo	Potassium citrate	189645	1
ACM	Potassium citrate	KNC0196J15	4
Caelo	Potassium citrate	15123102	2
Caelo	Potassium citrate	15148701	7
Euro OTC	Potassium citrate	1504024-01	2
Caelo	Potassium citrate	15123103	3
Caelo	Potassium citrate	15148706	9
Euro OTC	Potassium citrate	1509044-01	4
Caelo	Potassium citrate	15148702	1
Caelo	Potassium citrate	15148707	3
Caelo	Potassium citrate	15158706	1
Phoenix	Potassium citrate	15148708	1
Euro OTC	Potassium citrate	123456	6
Euro OTC	Potassium citrate	1603040-01	12
Caelo	Potassium citrate	12345678	1
Caelo	Potassium citrate	123654879	1
Caelo	Potassium citrate	12648	1
Caelo	Potassium citrate	12456	1
Phönix	Potassium citrate	15123103	1
Caelo	Potassium citrate	15435701	6
Caelo	Potassium citrate	151231	1
Caelo	Potassium citrate	154357025	1
Caelo	Potassium citrate	3012Q-01737	1
Caelo	Potassium citrate	gfte	1
Euro OTC	Potassium citrate	1915A-01737	1
Euro OTC	Potassium citrate	1606041-01	4
Caelo	Potassium citrate	1543702	1
Euro OTC	Potassium citrate	160601-01	1
Caelo	Potassium citrate	15435710	2
Euro OTC	Potassium citrate	160604-01	1
Sanacorp	Potassium citrate	160604101	1
Caelo	Potassium citrate	154357	3
Caelo	Potassium citrate	16113003	1
Caelo	Potassium citrate	15435709	2
Caelo	Potassium citrate	16113002	2
Euro OTC	Potassium citrate	1611017-01	3
Alliance	Potassium citrate	1611017-01	1
Caelo	Potassium citrate	15435702	1
Caelo	Potassium citrate	16113012	2
Caelo	Potassium citrate	16113008	1
Euro OTC	Potassium citrate	1705024-01	2
Euro OT/Phönix	Potassium citrate	3036325	1
Caelo	Potassium citrate	16113007	1
Caelo	Potassium citrate	16113006	1
Euro OTC	Potassium citrate	16113012	1

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Supplier	Substance	Batch	Spectra
Caelo	Potassium citrate	18007603	1

- 78 696 spectra from 565 *Apo-Ident* customers from a total of 26 047 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Potassium citrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Potassium citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	360	0	126 532
Type C	0	233	0	78 696

The substance/substance group *Potassium citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 97.4249 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20655	21936	4.02	46.84
21775	21936	3.71	47.24
21936	21936	0.00	46.70

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22476	22476	0.00	47.52
21452	22476	3.80	47.09
22921	22921	0.00	47.13

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Potassium hydrogen tartrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20509-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Potassium hydrogen tartrate; Kalii hydrogentartras

Special notes

When selecting the *Potassium hydrogen tartrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Potassium hydrogen tartrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potassium hydrog...	11345805	20772	40	20120103
Caelo	Potassium hydrog...	15354609	23193	40	20151030
Caelo	Potassium hydrog...	170656	23285	40	20170511*

Validation samples

A total of 280317 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 *Potassium hydrogen tartrate*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 *Potassium hydrogen tartrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Potassium hydrogen tartrate	11345805	20644	40
Caelo	Potassium hydrogen tartrate	11345805	20645	40
Caelo	Potassium hydrogen tartrate	17065604	23414	40
Caelo	Potassium hydrogen tartrate	17065603	23709	40

- 126732 spectra from a total of 2786 batches from further 781 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 20 *Apo-Ident* customers from 18 batches from the substance/substance group *Potassium hydrogen tartrate*.

*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
Caelo	Potassium hydrogen tartrate	11127417	1
Caelo	Potassium hydrogen tartrate	11345807	1
Gehe	Potassium hydrogen tartrate	11345808	1
Caelo	Potassium hydrogen tartrate	13030006	2
Caelo	Potassium hydrogen tartrate	17061303	1
Caelo	Potassium hydrogen tartrate	90573259	1
Caelo	Potassium hydrogen tartrate	13133104	2
Caelo	Potassium hydrogen tartrate	160514b	1
Caelo	Potassium hydrogen tartrate	13133114	1
Caelo	Potassium hydrogen tartrate	13133120	2
Caelo	Potassium hydrogen tartrate	14115208	1
Sanacorp	Potassium hydrogen tartrate	14115208	3
Caelo	Potassium hydrogen tartrate	23062015A	1
Caelo	Potassium hydrogen tartrate	15081005	1
Caelo	Potassium hydrogen tartrate	15081008	2
phönix	Potassium hydrogen tartrate	15354604	1
Caelo	Potassium hydrogen tartrate	15081010	1
Sanacorp	Potassium hydrogen tartrate	15354609	1
Caelo	Potassium hydrogen tartrate	15354604	2
Caelo	Potassium hydrogen tartrate	1534609	1
Caelo	Potassium hydrogen tartrate	15354609	1

- 78 901 spectra from 565 *Apo-Ident* customers from a total of 26 119 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Potassium hydrogen tartrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Potassium hydrogen tartrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	0	126 732
Type C	0	27	1	78 901

The substance/substance group *Potassium hydrogen tartrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	96.4286 % (> 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
20772	23285	6.11	58.03
23193	23285	2.93	59.14
23285	23285	0.00	59.69

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Potassium sodium tartrate tetrahydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20782-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Potassium sodium tartrate tetrahydrate; Kalii natrii tartras tetrahydricus

Special notes

When selecting the *Potassium sodium tartrate tetrahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Potassium sodium tartrate tetrahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potassium sodium...	12030207	20782	40	20120213
Caelo	Potassium sodium...	13216605	20998	40	1404530
Caelo	Potassium sodium...	14376001	21801	40	20150204

Validation samples

A total of 280 317 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 *Potassium sodium tartrate tetrahydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Potassium sodium tartrate tetrahydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Potassium sodium tartrate te...	14376001	21801 [†]	20
Caelo	Potassium sodium tartrate te...	15375607	23207	40
Caelo	Potassium sodium tartrate te...	172577	23824	40

- 126 792 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 4 *Apo-Ident* customers from 1 batches from the substance/substance group *Potassium sodium tartrate tetrahydrate*.

Supplier	Substance	Batch	Spectra
Caelo	Potassium sodium tartrate te...	15375601	12

[†]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*.

- 78 917 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Potassium sodium tartrate tetrahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Potassium sodium tartrate tetrahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	12	0	78 917

The substance/substance group *Potassium sodium tartrate tetrahydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8818 %)	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
20782	20998	4.54	44.25
20998	20998	0.00	44.03
21801	20998	5.94	44.12

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Potassium sorbate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20020-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Potassium sorbate; Kalii sorbas

Special notes

When selecting the *Potassium sorbate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Potassium sorbate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potassium sorbate	13224604	21444	40	20130813
Euro OTC	Potassium sorbate	1508025	21892	40	20150902*
Euro OTC	Potassium sorbate	1608013	22786	40	20160819*
Caelo	Potassium sorbate	163266	23059	40	20170105*
Caelo	Potassium sorbate	17170008	23585	30	20170711

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 190 spectra of 5 reference samples from the substance/substance group *Potassium sorbate*. These samples are listed above in the [calibration samples](#) section.
- 74 306 spectra from a total of 1618 batches from further 372 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 [†].

- 280 spectra of 8 reference samples from the substance/substance group *Potassium sorbate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Potassium sorbate	13224604	21444 [†]	20
Euro OTC	Potassium sorbate	1508025	21892 [†]	20
Euro OTC	Potassium sorbate	1703034	23176	40
Caelo	Potassium sorbate	171700	23638	40
Euro OTC	Potassium sorbate	1710015	23772	40
Caelo	Potassium sorbate	173451	23830	40
Euro OTC	Potassium sorbate	1805029	24126	40
Caelo	Potassium sorbate	181650	24224	40

- 126 612 spectra from a total of 2781 batches from further 781 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.

- 567 spectra from 320 *Apo-Ident* customers from 123 batches from the substance/substance group *Potassium sorbate*.

Supplier	Substance	Batch	Spectra
Caelo	Potassium sorbate	10012210	1
Caelo	Potassium sorbate	11214207	1
Spinnrad GmbH	Potassium sorbate	111033102	1
Caelo	Potassium sorbate	10199505	1
Gehe	Potassium sorbate	11261304	1
Caelo	Potassium sorbate	11261304	2
Caelo	Potassium sorbate	12059908	2
	Potassium sorbate	10012203	1
Caelo	Potassium sorbate	12345	1
Caelo	Potassium sorbate	12059909	4
Caelo	Potassium sorbate	1205999	1
Euro OTC	Potassium sorbate	1111038-01	1
Caesar & Loretz GmbH	Potassium sorbate	11261303	1
Caelo	Potassium sorbate	12059905	2
Caelo	Potassium sorbate	12211101	8
Caelo	Potassium sorbate	3512M-01748	1
Spinnrad	Potassium sorbate	111033102	1
Spinnrad	Potassium sorbate	312331021	2
Caelo	Potassium sorbate	20021112-2	1
Spinnrad GmbH	Potassium sorbate	912331023	2
Sanacorp	Potassium sorbate	12211101	1
s.Prüfprotokoll	Potassium sorbate		1
Caelo	Potassium sorbate	12211107	15
Caelo	Potassium sorbate	12059914	2
Caelo	Potassium sorbate	91623299	2
Noweda	Potassium sorbate	12211101	1
Caelo	Potassium sorbate	12211102	4
Anzag	Potassium sorbate	12211107	1
Caelo	Potassium sorbate	13065204	11
Spinnrad	Potassium sorbate	912331023	4
Caelo	Potassium sorbate	12211108	2
Caelo	Potassium sorbate	912331023	1
Caelo	Potassium sorbate	12211121	4
Caelo	Potassium sorbate	K-010213-1	1
Caesar/Lorenz	Potassium sorbate	13065204	1
Caelo	Potassium sorbate	13065205	12
Caelo	Potassium sorbate	1112331024	1
Euro OTC	Potassium sorbate	1111038-02	2
siehe WE-Prüfprotokoll	Potassium sorbate	61/11	1
Gehe	Potassium sorbate	13065205	1
Phoenix	Potassium sorbate	1397235	1
canea, gehe	Potassium sorbate	13065215	1
Caelo	Potassium sorbate	AKD10	1
AHD	Potassium sorbate	13065216	1
Caelo	Potassium sorbate	13065216	11
Euro OTC	Potassium sorbate	111103802	1
Caelo	Potassium sorbate	12211123	1
Caelo	Potassium sorbate	9305601	2
Caelo	Potassium sorbate	13065217	11
Gehe	Potassium sorbate	13065216	1
Caelo	Potassium sorbate	12059902	1
Caelo	Potassium sorbate	200613K1	1
Caelo	Potassium sorbate	13065211	1
Sanacorp	Potassium sorbate	13065217	1

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Supplier	Substance	Batch	Spectra
Noweda	Potassium sorbate	13065222	1
Caelo	Potassium sorbate	11192305	3
Sonnenberg-Apotheke	Potassium sorbate	13224604	1
Caelo	Potassium sorbate	13224604	16
Caelo	Potassium sorbate	13065222	1
Fagron	Potassium sorbate	13065217	1
Caesar & Loretz GmbH Hi...	Potassium sorbate	13065217	2
Caelo	Potassium sorbate	13277804	1
Ichthyol/Noweda	Potassium sorbate	13224604	1
Euro OTC	Potassium sorbate	1312024-01	2
Fagron	Potassium sorbate	3912A-01748	1
Caelo	Potassium sorbate	13224611	11
Caelo	Potassium sorbate	13224608	2
Caelo	Potassium sorbate	13111409	1
Apomix/Noweda	Potassium sorbate	13224611	1
Sanacorp	Potassium sorbate	13224611	1
Caelo	Potassium sorbate	1312024-01	2
Caelo	Potassium sorbate	13224612	16
Spinnrad GmbH	Potassium sorbate	1114331022	1
Anzag 12.01.15	Potassium sorbate	13224611	1
Caelo	Potassium sorbate	13224610	1
Euro OTC	Potassium sorbate	13224612	1
Spinnrad	Potassium sorbate	1114331022	3
spinnrad	Potassium sorbate	1114331022	1
Caelo	Potassium sorbate	14380601	17
Fagron	Potassium sorbate	1114331022	1
Caelo	Potassium sorbate	14380607	3
Fresenius	Potassium sorbate	220214221	1
Caelo	Potassium sorbate	14192605	2
Caelo	Potassium sorbate	14380606	7
Fagron	Potassium sorbate	4314U-01748	1
Caelo	Potassium sorbate	1438060	2
Caelo	Potassium sorbate	14380602	2
Spinnrad	Potassium sorbate	214331021	1
Caelo	Potassium sorbate	14380610	11
Caesar&Loretz GmbH/Sana...	Potassium sorbate	14380607	1
Caelo	Potassium sorbate		1
Spinnrad/Gehe	Potassium sorbate	315331021	1
Caelo	Potassium sorbate	14380612	2
Caelo	Potassium sorbate	15248204	16
Euro OTC	Potassium sorbate	1508025-01	7
Caelo	Potassium sorbate	15248205	10
Sanacorp	Potassium sorbate	14380610	1
Caelo	Potassium sorbate	14380622	8
Caelo	Potassium sorbate	14380621	9
Caelo	Potassium sorbate	14380627	7
Caelo	Potassium sorbate	15248203	3
Caelo	Potassium sorbate	15382105	9
Spinnrad	Potassium sorbate	315331021	2
Caelo	Potassium sorbate	14380620	6
Fagron	Potassium sorbate	14380622	1
Caesar & Loretz GmbH	Potassium sorbate	14380627	1
Caelo	Potassium sorbate	14380613	1
Caelo	Potassium sorbate	14380632	15
Caesar&Loretz GmbH	Potassium sorbate	14380622	1
Euro OTC	Potassium sorbate	216331021	1
Bombastus	Potassium sorbate	14380632	1
Spinnrad	Potassium sorbate	815331022	2
spinnrad	Potassium sorbate	216331021	1
Caelo	Potassium sorbate	143806	1

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Supplier	Substance	Batch	Spectra
Spinnrad - Noweda	Potassium sorbate	315331021	1
Fagron	Potassium sorbate	3115M-01748	1
Caelo	Potassium sorbate	14380633	11
Spinnrad GmbH	Potassium sorbate	214331021	1
phönix	Potassium sorbate	14380632	1
spinnrad/gehe	Potassium sorbate	216331021	1
Caesar & Loretz/Noweda	Potassium sorbate	14380621	1
Caelo	Potassium sorbate	14380635	7
Spinnrad	Potassium sorbate	216331021	1
Euro OTC	Potassium sorbate	14380622	1
Caelo	Potassium sorbate	15382114	6
Caelo	Potassium sorbate	16156505	1
Phoenix	Potassium sorbate	14380627	1
Caelo	Potassium sorbate	15382103	1
Gehe / Spinnrad	Potassium sorbate	216331021	1
Phoenix	Potassium sorbate	216331021	1
Alliance Healthcare	Potassium sorbate	15382115	1
Anzag	Potassium sorbate	15382114	2
Caelo	Potassium sorbate	15382115	3
Noweda / Spinnrad	Potassium sorbate	216331021	1
Caelo	Potassium sorbate	16326607	11
Caelo	Potassium sorbate	14380618	1
Caelo	Potassium sorbate	16326606	9
Noweda	Potassium sorbate	15382115	1
Euro OTC	Potassium sorbate	15382115	1
Spinnrad/Sannacorp	Potassium sorbate	616331022	1
Caelo	Potassium sorbate	16326602	2
Spinnrad	Potassium sorbate	616331022	2
cealo	Potassium sorbate	16326607	1
Gehe	Potassium sorbate	16326606	1
Kehr	Potassium sorbate	16326607	1
spinnrad GmbH	Potassium sorbate	616331022	1
Phönix	Potassium sorbate	16326607	1
Caelo	Potassium sorbate	16326608	10
Caelo	Potassium sorbate	16326609	10
Caelo	Potassium sorbate	15382106	1
phönix	Potassium sorbate	16326608	1
GEHE	Potassium sorbate	17170008	1
Caelo	Potassium sorbate	17170008	12
Caelo	Potassium sorbate	27101705	1
Caelo	Potassium sorbate	17170007	10
Jenne	Potassium sorbate	17170007	1
Caelo	Potassium sorbate	17170007-20171106Ma1	1
Sanacorp	Potassium sorbate	17170007	1
Spinnrad	Potassium sorbate	317331021	3
Caelo	Potassium sorbate	17170005	1
Caelo	Potassium sorbate	17170002	3
Caelo	Potassium sorbate	14140007	1
Noweda	Potassium sorbate	16326606	1
WE: über Eyach 5g/2,87E...	Potassium sorbate	14380601	1
Caelo	Potassium sorbate	1608013-01	1
Caelo	Potassium sorbate	16326615	1
gehe	Potassium sorbate	17170014	1
Caesar&Loretz GmbH	Potassium sorbate	17170014	1
p&m cosmetics/gehe	Potassium sorbate	17170014	1
Caelo	Potassium sorbate	17170013	6
Caelo	Potassium sorbate	17170006	1
Caelo	Potassium sorbate	17170014	8
Gehe	Potassium sorbate	17170013	1
Caelo	Potassium sorbate	17170012	2

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Supplier	Substance	Batch	Spectra
Cealo	Potassium sorbate	1710013	1
Euro OTC	Potassium sorbate	17170013	1
Kehr/Spinnrad	Potassium sorbate	317331021	1
Cealo	Potassium sorbate	90318101	1
Phönix/Spinnrad	Potassium sorbate	1117331022	1
Cealo	Potassium sorbate	17170017	4
Spinnrad/Noweda	Potassium sorbate	1117331022	1
Allianz	Potassium sorbate	17170006	1
Cealo	Potassium sorbate	17345103	7
Cealo	Potassium sorbate	17345105	1
Cealo	Potassium sorbate	9061806	1
Euro OTC	Potassium sorbate	180529-01	1
	Potassium sorbate	17170017	1
Cealo	Potassium sorbate	17345104	7
Spinrad/Phönix	Potassium sorbate	218331021	1
Cealo/ Noweda	Potassium sorbate	17345103	1
Cealo	Potassium sorbate	7111805	1
Bombastus	Potassium sorbate	1117331022	1
Cealo	Potassium sorbate	17345116	5
Cealo	Potassium sorbate	18165006	2
Kehr	Potassium sorbate	18165006	1
Cealo	Potassium sorbate	317331021	1

- 78 362 spectra from 565 *Apo-Ident* customers from a total of 26 018 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Potassium sorbate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Potassium sorbate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	190	0	74 306
Type B	0	250	30	126 612
Type C	0	498	69	78 362

The substance/substance group *Potassium sorbate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.8421 %)
Type B	100.0000 % (> 99.9901 %)	89.2857 % (> 88.2143 %)
Type C	100.0000 % (> 99.8817 %)	87.8307 % (> 87.3016 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
23059	23059	0.00	58.20
23585	23059	7.99	57.10
21444	21892	9.96	56.72
21892	21892	0.00	55.92
22786	22786	0.00	53.63

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Potassium tartrate hemihydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20999-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Potassium tartrate hemihydrate; Kalii tartras hemihydricus

Special notes

When selecting the *Potassium tartrate hemihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Potassium tartrate hemihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potassium tartra...	13331104	21440	40	20131002
Caelo	Potassium tartra...	15167701	21812	40	20150608
Caelo	Potassium tartra...	160289	22462	40	20160405*

Validation samples

A total of 280317 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 *Potassium tartrate hemihydrate*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 5 reference samples from the substance/substance group *Potassium tartrate hemihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Potassium tartrate hemihydrate	13331101	20999	40
Caelo	Potassium tartrate hemihydrate	13331104	21440 [†]	20
Caelo	Potassium tartrate hemihydrate	15167701	21812 [†]	20
Caelo	Potassium tartrate hemihydrate	160289	22462 [†]	20
Caelo	Potassium tartrate hemihydrate	182203	24248	40

- 126752 spectra from a total of 2784 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 3 *Apo-Ident* customers from 11 batches from the substance/substance group *Potassium tartrate hemihydrate*.

*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	Potassium tartrate hemihydrate	11225007	1
Caelo	Potassium tartrate hemihydrate	27061304	1
Caelo	Potassium tartrate hemihydrate	12322110	1
Caelo	Potassium tartrate hemihydrate	13331113	1
Caelo	Potassium tartrate hemihydrate	13111415	1
Caelo	Potassium tartrate hemihydrate	15167703	1
Caelo	Potassium tartrate hemihydrate	24061705	1
Caelo	Potassium tartrate hemihydrate	17176002	2
Caelo	Potassium tartrate hemihydrate	17176004	1
Caelo	Potassium tartrate hemihydrate	19051804	1
Caelo	Potassium tartrate hemihydrate	17176007	1

- 78 917 spectra from 565 *Apo-Ident* customers from a total of 26 126 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Potassium tartrate hemihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Potassium tartrate hemihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	137	3	126 752
Type C	0	12	0	78 917

The substance/substance group *Potassium tartrate hemihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	97.8571 % (> 95.7143 %)
Type C	100.0000 % (> 99.8818 %)	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
21812	22462	3.15	42.15
21440	22462	3.77	41.43
22462	22462	0.00	45.12

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Povidone 25, soluble**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20684-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Povidone 25, soluble; Povidonum 25, solubile

Special notes

When selecting the *Povidone 25, soluble* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Povidone 25, soluble*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Povidone 25, sol. ...	12032714	20684	40	1402437
Fagron	Povidone 25, sol. ...	12E22-N05	20770	40	1411537
Caelo	Povidone 25, sol. ...	14142103	21378	40	AR-15-FG-000596-01
Fagron	Povidone 25, sol. ...	13J21-N02	22731	40	AR-16-FG-019116-01
Caelo	Povidone 25, sol. ...	16307808	23255	40	AR-17-FG-015299-02
Fagron	Povidone 25, sol. ...	15C12-B02-323006	23265	40	1710348
Caelo	Povidone 25, sol. ...	180276	24044	40	20180202*

Validation samples

A total of 280 317 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 *Povidone 25, soluble*. These samples are listed above in the [calibration samples](#) section.
- 74 216 spectra from a total of 1616 batches from further 372 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 *Povidone 25, soluble*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Povidone 25, soluble	172091	23619	40
Caelo	Povidone 25, soluble	180766	24245	40
Caelo	Povidone 25, soluble	181820	24246	40
Caelo	Povidone 25, soluble	182383	24291	40
Caelo	Povidone 25, soluble	183000	24396	40

- 126 692 spectra from a total of 2784 batches from further 781 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 20 *Apo-Ident* customers from 30 batches from the substance/substance group *Povidone 25, soluble*.

*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
Caelo	Povidone 25, soluble	12376301	1
Fagron	Povidone 25, soluble	11276509T0	1
Caelo	Povidone 25, soluble	12032714	1
Caelo	Povidone 25, soluble	13323407	2
Caelo	Povidone 25, soluble	14142109	3
Caelo	Povidone 25, soluble	14142103	1
Caelo	Povidone 25, soluble	14207508	3
Caelo	Povidone 25, soluble	14207511	4
Fagron	Povidone 25, soluble	24701988Q0	1
Caelo	Povidone 25, soluble	14207517	1
Caelo	Povidone 25, soluble	15383103	1
Caelo	Povidone 25, soluble	14207515	1
Caelo	Povidone 25, soluble	15383101	3
Caelo	Povidone 25, soluble	15383102	1
Caelo	Povidone 25, soluble	16051102	1
Caelo	Povidone 25, soluble	16051104	1
Caelo	Povidone 25, soluble	16051101	1
Caelo	Povidone 25, soluble	16051108	1
Caelo	Povidone 25, soluble	16051110	1
Fagron	Povidone 25, soluble	15C12-B02-327866	1
Alliance	Povidone 25, soluble	16307808	1
Caelo	Povidone 25, soluble	163078085328	1
Caelo	Povidone 25, soluble	16307809	2
Caelo	Povidone 25, soluble	16307812	1
Caelo	Povidone 25, soluble	16307811	1
Caelo	Povidone 25, soluble	17209104	3
Alliance	Povidone 25, soluble	17209106	1
Caelo	Povidone 25, soluble	18024602	1
Caelo	Povidone 25, soluble	18027602	2
Caelo	Povidone 25, soluble	18112201	2
Alliance	Povidone 25, soluble	18112201	1

- 78 883 spectra from 565 *Apo-Ident* customers from a total of 26 108 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Povidone 25, 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 *Povidone 25, 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	280	0	74 216
Type B	0	158	42	126 692
Type C	0	41	5	78 883

The substance/substance group *Povidone 25, 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 % (> 99.9887 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9901 %)	79.0000 % (> 77.5000 %)
Type C	100.0000 % (> 99.8817 %)	89.1304 % (> 82.6087 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20684	20684	0.00	16.36
20770	20770	0.00	18.45
21378	21378	0.00	13.42
23255	23255	0.00	14.63
23265	23265	0.00	26.00
22731	22731	0.00	22.15
24044	24044	0.00	20.35

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Povidone iodine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20472-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Povidone iodine; Povidonum iodinatum

Special notes

When selecting the *Povidone iodine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Povidone iodine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Povidone iodine	13337205	21466	40	20131021
Euro OTC	Povidone iodine	1501029-01	21777	40	20150211
Euro OTC	Povidone iodine	1509009	21908	40	20150918*
Caelo	Povidone iodine	15234101	23252	40	AR-17-FG-015433-02
Euro OTC	Povidone iodine	1606026-02	23906	40	20160708
Euro OTC	Povidone iodine	1805007	24118	40	20180525*

Validation samples

A total of 280 317 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 *Povidone iodine*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 9 reference samples from the substance/substance group *Povidone iodine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Povidone iodine	1110013-02	21073	40
Caelo	Povidone iodine	13337205	21466 [†]	20
Euro OTC	Povidone iodine	1501029-01	21777 [†]	20
Euro OTC	Povidone iodine	1509009	21908 [†]	20
Euro OTC	Povidone iodine	1606026	22675	40
Caelo	Povidone iodine	15234109	23256	40
Euro OTC	Povidone iodine	1704007	23435	40
Caelo	Povidone iodine	182385	24234	40
Caelo	Povidone iodine	180763	24261	40

- 126 592 spectra from a total of 2780 batches from further 781 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.

- 53 spectra from 23 *Apo-Ident* customers from 30 batches from the substance/substance group *Povidone iodine*.

Supplier	Substance	Batch	Spectra
Caelo	Povidone iodine	12072605	1
Caelo	Povidone iodine	11168607	1
Stumpf	Povidone iodine	11168612	1
Euro OTC	Povidone iodine	1110013-02	4
Caelo	Povidone iodine	12153106	2
Euro OTC	Povidone iodine	111001302	1
Euro OTC	Povidone iodine	110013-02	1
Caelo	Povidone iodine	1110013-02	1
Caelo	Povidone iodine	11168612	1
BASF, Noweda	Povidone iodine	1110013-02	1
Noweda	Povidone iodine	G0354BPZ0	1
Caelo	Povidone iodine	12153110	2
Caelo	Povidone iodine	19061302	1
Caelo	Povidone iodine	12153116	2
Caelo	Povidone iodine	12153119	2
Phönix	Povidone iodine	1110013-02	1
Euro OTC	Povidone iodine	1407032-01	5
Fagron	Povidone iodine	1110013-02	1
Euroo/Phoenix	Povidone iodine	G3115BPZ0	1
Euro OTC	Povidone iodine	130901001	1
Caelo	Povidone iodine	15121402	1
Caelo	Povidone iodine	14195810	2
Euroo/Sana	Povidone iodine	1501029-01	3
Euro OTC	Povidone iodine	G4208BPZ0	2
Euro OTC	Povidone iodine	1509009-01	1
Euro OTC	Povidone iodine	1401029-01	1
Caelo	Povidone iodine	15234101	1
Euro OTC	Povidone iodine	1509009-02	1
Euro OTC	Povidone iodine	1603023-01	2
Caelo	Povidone iodine	15442405	1
Caelo	Povidone iodine	15234109	1
Euro OTC	Povidone iodine	1606026	1
Euro OTC	Povidone iodine	1704007-01	2
Euro OTC	Povidone iodine	1606026-02	2
Euro OTC	Povidone iodine	8051808	1

- 78 876 spectra from 565 *Apo-Ident* customers from a total of 26 108 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Povidone iodine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Povidone iodine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	229	71	126 592
Type C	0	36	17	78 876

The substance/substance group *Povidone iodine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	76.3333 % (> 75.3333 %)
Type C	100.0000 % (> 99.8817 %)	67.9245 % (> 62.2642 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21777	21908	5.35	22.54
23906	21908	8.29	21.63
23252	23252	0.00	19.56
21466	21908	4.82	23.71
24118	24118	0.00	39.86
21908	21908	0.00	23.05

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Prasterone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20703-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Prasterone; Prasteronum

Special notes

When selecting the *Prasterone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Prasterone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prasterone	1102036-01	20703	40	1404310
Fagron	Prasterone	13J10-B02-287175	20960	40	1404309
Euro OTC	Prasterone	1506011	21824	40	20150629*
Fagron	Prasterone	15G14-B07-310827	21917	40	20150814
Euro OTC	Prasterone	1602018	22506	30	20160301*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prasterone	1704012	23389	40	20170529*
Euro OTC	Prasterone	1707014	23695	40	20170829*
Fagron	Prasterone	16L13-B01-330724	23865	40	20161228
Euro OTC	Prasterone	1710035	23868	40	20171212*
Euro OTC	Prasterone	1712014	23893	40	20180115*
Audor	Prasterone	APZDHA16003-M	23931	40	1805404

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 430 spectra of 11 reference samples from the substance/substance group *Prasterone*. These samples are listed above in the [calibration samples](#) section.
- 74 066 spectra from a total of 1612 batches from further 372 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 [†].

- 640 spectra of 16 reference samples from the substance/substance group *Prasterone*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Prasterone	1506011	21824 [†]	20
Fagron	Prasterone	15G14-B07-310827	21917 [†]	20
Euro OTC	Prasterone	1702025	23147	40
Audor Pharma	Prasterone	APZDHA16003-1MD	23932	40
Fagron	Prasterone	18C12-B01-347633	23990	40
Euro OTC	Prasterone	1805018	24137	40
Euro OTC	Prasterone	1809010	24318	40
Euro OTC	Prasterone	1809009	24323	40
Audor Pharma	Prasterone	APZDHAC17003MD	24412	40
Audor Pharma	Prasterone	APZDHAC18004D	24430	40
Euro OTC	Prasterone	1901030	24453	40
Euro OTC	Prasterone	1901031	24454	40
Euro OTC	Prasterone	1506011	21824SI	60
Fagron	Prasterone	15G14-B07-310827	21917SI	60
Euro OTC	Prasterone	1602018	22506SI	40
Euro OTC	Prasterone	1702025	23147SI	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.

- 126 252 spectra from a total of 2776 batches from further 781 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.

- 89 spectra from 28 *Apo-Ident* customers from 57 batches from the substance/substance group *Prasterone*.

Supplier	Substance	Batch	Spectra
Fagron	Prasterone	12G04-N19	2
Fragon	Prasterone	12G04-N19	1
Audor Pharma	Prasterone	10050051/1P	1
Euro OTC	Prasterone	1203010-01	1
Euro OTC	Prasterone	22021306	1
Fagron	Prasterone	12C26-N09	1
Fagron	Prasterone	19061304	1
Fagron	Prasterone	12K30-N06	3
Euro OTC	Prasterone	2081302	1
Audor Pharma	Prasterone	AP11040002P	2
Haihang	Prasterone	20130507	1
Euro OTC	Prasterone	1306021-01	3
Euro OTC	Prasterone	9215-4/09	1
Haihang Industry	Prasterone	20130816	4
Euro OTC	Prasterone	XPC0263	1
Fagron	Prasterone	13J10-B02-287177	1
Euro OTC	Prasterone	1311002-01	2
Nachprüfung	Prasterone	120022	1
Fagron	Prasterone	7013260004	1
Fagron	Prasterone	13J10-B02	1
Euro OTC	Prasterone	1401040-01	1
Fagron	Prasterone	14C18-B02	1
Fagron	Prasterone	14C18-B02-293606	1
Fagron	Prasterone	14C18-Bo2-293603	1
Fagron	Prasterone	14C18-B02-293602	1
Euro OTC	Prasterone	1409004-01	4
Fagron	Prasterone	14c18b02293602	1
Fagron	Prasterone	14h12b05-297723	1
Fagron	Prasterone	14H12-B05-297727	2
Euro OTC	Prasterone	5101849	1
Euro OTC	Prasterone	26031506	1
Euro OTC	Prasterone	T03-04/1412028-01	1
Euro OTC	Prasterone	30041509	1
Euro OTC	Prasterone	1412028-01	4
Euro OTC	Prasterone	4091511	1
Euro OTC	Prasterone	1506011-01	3
Caelo	Prasterone	1412028-01	1
NWM Shandong Northwest ...	Prasterone	PST151207	1
Fagron	Prasterone	15A15-B40-307323	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	Prasterone	15G14-B07-310827	1
Euro OTC	Prasterone	1602018-01	3
Euro OTC	Prasterone	1602018-02	2
EuRho	Prasterone	1311002-01	1
Caelo	Prasterone	16B19-B04-318665	1
Fagron	Prasterone	16B19-B04-322246	1
Euro OTC	Prasterone	23021711	1
Fagron	Prasterone	15I18-B09-316798	1
Fargon	Prasterone	16B19-B04-318665	1
Fargon	Prasterone	16J26-B03-327602	1
Caelo	Prasterone	16I02-B02-326485	1
Euro OTC	Prasterone	1702025	1
Caelo	Prasterone	16I02-B02-326485	2
Fagron	Prasterone	16B19-B04-318665	2
Euro OTC	Prasterone	1412028	1
Fagron	Prasterone	27071705	1
Euro OTC	Prasterone	1702025-01	4
Euro OTC	Prasterone	170202501	1
Audor Pharma	Prasterone	APZDHAC17003-MD	1
Fagron	Prasterone	18B02-B02-345147	1
Fargon	Prasterone	18C12	1
Audor Pharma	Prasterone	APZDHA16003-M	1
Fagron	Prasterone	18B13-B09346424	1

- 78 840 spectra from 565 *Apo-Ident* customers from a total of 26 080 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Prasterone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prasterone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	430	0	74 066
Type B	0	534	106	126 252
Type C	0	82	7	78 840

The substance/substance group *Prasterone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.6047 %)
Type B	100.0000 % (> 99.9901 %)	83.4375 % (> 82.9688 %)
Type C	100.0000 % (> 99.8817 %)	92.1348 % (> 88.7640 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22506	22506	0.00	47.03
20703	20703	0.00	43.49
20960	20960	0.00	42.48
23389	23389	0.00	31.47
23868	23868	0.00	27.86
21824	21824	0.00	42.47
23695	23695	0.00	36.49
23893	23893	0.00	31.88
23931	23931	0.00	37.50
21917	21824	11.51	39.36
23865	23695	10.99	45.83

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Prednicarbate, micronized**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20196-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Prednicarbate, micronized; Prednicarbatum micronisatum

Special notes

When selecting the *Prednicarbate, micronized* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Prednicarbate, micronized*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Prednicarbate, m...	12D27-N04	20700	40	20120509
Caelo	Prednicarbate, m...	13119402	20832	60	1501576
Caelo	Prednicarbate, m...	13119402	20833	60	20130517
Caelo	Prednicarbate, m...	13372404	21368	50	AR-15-FG-007941-02
Caelo	Prednicarbate, m...	13372404	21369	49	20131119

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Prednicarbate, m...	14A27-B02-291256	21572	40	AR-16-FG-011442-01
Euro OTC	Prednicarbate, m...	1302033-02	21610	40	1509286
Euro OTC	Prednicarbate, m...	1507011	21858	40	20150730*
Euro OTC	Prednicarbate, m...	1601058	22366	30	20160223*
Fagron	Prednicarbate, m...	12D27-N04	20700SI	33	20120509
Caelo	Prednicarbate, m...	13119402	20833SI	20	20130517
Caelo	Prednicarbate, m...	13372404	21369SI	23	20131119
Euro OTC	Prednicarbate, m...	1601058	22366SI	21	20160223*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 506 spectra of 13 reference samples from the substance/substance group *Prednicarbate, micronized*. These samples are listed above in the [calibration samples](#) section.
- 73990 spectra from a total of 1616 batches from further 372 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 [†].

- 870 spectra of 32 reference samples from the substance/substance group *Prednicarbate, micronized*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Prednicarbate, micronized	14A27-B02-291256	21572 [†]	20
Euro OTC	Prednicarbate, micronized	1302033-02	21610 [†]	20
Euro OTC	Prednicarbate, micronized	1507011	21858 [†]	20
Euro OTC	Prednicarbate, micronized	1601058	22366 [†]	15
Caelo	Prednicarbate, micronized	160874	22447	60
Euro OTC	Prednicarbate, micronized	1605001	22558	30
Euro OTC	Prednicarbate, micronized	1607012	22703	40
Euro OTC	Prednicarbate, micronized	1609022	22860	40
Caelo	Prednicarbate, micronized	170138	23040	40
Euro OTC	Prednicarbate, micronized	1707022	23540	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	Prednicarbate, micronized	173156	23845	40
Caelo	Prednicarbate, micronized	172204	23848	40
Euro OTC	Prednicarbate, micronized	1801013	23887	40
Euro OTC	Prednicarbate, micronized	1805005	24134	40
Euro OTC	Prednicarbate, micronized	1809015	24320	40
Fagron	Prednicarbate, micronized	12D27-N04	20700SI [†]	15
Caelo	Prednicarbate, micronized	13119402	20833SI [†]	10
Caelo	Prednicarbate, micronized	13372404	21369SI [†]	10
Fagron	Prednicarbate, micronized	14A27-B02-291256	21572SI	36
Euro OTC	Prednicarbate, micronized	1507011	21858SI	15
Euro OTC	Prednicarbate, micronized	1601058	22366SI [†]	10
Caelo	Prednicarbate, micronized	160874	22447SI	30
Euro OTC	Prednicarbate, micronized	1605001	22558SI	25
Euro OTC	Prednicarbate, micronized	1607012	22703SI	28
Euro OTC	Prednicarbate, micronized	1609022	22860SI	27
Caelo	Prednicarbate, micronized	170138	23040SI	20
Euro OTC	Prednicarbate, micronized	1707022	23540SI	19
Caelo	Prednicarbate, micronized	173156	23845SI	20
Caelo	Prednicarbate, micronized	172204	23848SI	20
Euro OTC	Prednicarbate, micronized	1801013	23887SI	20
Euro OTC	Prednicarbate, micronized	1805005	24134SI	20
Euro OTC	Prednicarbate, micronized	1809015	24320SI	20

- 126 022 spectra from a total of 2771 batches from further 781 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.

- 561 spectra from 240 *Apo-Ident* customers from 160 batches from the substance/substance group *Prednicarbate, micronized*.

Supplier	Substance	Batch	Spectra
Fagron	Prednicarbate, micronized	11L23-N07	3
Caelo	Prednicarbate, micronized	C0333/1111070	1
Fagron	Prednicarbate, micronized	12D27-N04	3
Defektur	Prednicarbate, micronized	12D27-N04	1
Fagron	Prednicarbate, micronized	12B20-N06	2
Gehe	Prednicarbate, micronized	12B14-N02	1
Sanacorp	Prednicarbate, micronized	11L23-N07	1
Caelo	Prednicarbate, micronized	11L23-N07	1
Caelo	Prednicarbate, micronized	12383301	1
Fagron	Prednicarbate, micronized	13C25-N06	6
Fagron	Prednicarbate, micronized	13C25-N02	1
Fagron	Prednicarbate, micronized	7061303	1
Fagron	Prednicarbate, micronized	13F11-N01	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
Fagron	Prednicarbate, micronized	13c25-no6	1
Fagron	Prednicarbate, micronized	9G14-N06	1
Fagron	Prednicarbate, micronized	9E04-N02	1
Fagron	Prednicarbate, micronized	13G05-N03	4
Caelo	Prednicarbate, micronized	13224401	5
Fagron	Prednicarbate, micronized	13/23-N04	3
Caelo	Prednicarbate, micronized	12383309	1
Fagron	Prednicarbate, micronized	13I23-N04	6
Euro OTC	Prednicarbate, micronized	1302033-02	2
Caelo	Prednicarbate, micronized	13119401	1
Sino Phyto	Prednicarbate, micronized	13224401	1
Fagron	Prednicarbate, micronized	NT0555M13I23-N04	1
Caelo	Prednicarbate, micronized	13372403	9
Caelo	Prednicarbate, micronized	13119402	1
Caelo	Prednicarbate, micronized	13/23-N04	1
Caelo	Prednicarbate, micronized	13224406	1
Fagron	Prednicarbate, micronized	14A27-B02-291256	12
Euro OTC	Prednicarbate, micronized	1302033-01	1
Caelo	Prednicarbate, micronized	13372410	6
Caelo	Prednicarbate, micronized	9764897	1
Fagron	Prednicarbate, micronized	13372408	1
Fagron	Prednicarbate, micronized	14A27-B02-291258	2
Fagron	Prednicarbate, micronized	14a27-b02-291256	2
Fagron	Prednicarbate, micronized	14B13-B31-291255	1
Apomix/Noweda	Prednicarbate, micronized	13372410	2
Caelo	Prednicarbate, micronized	13372419	4
Caelo	Prednicarbate, micronized	13372408	1
Newchem spa/Noweda	Prednicarbate, micronized	14A27-B02-291256	1
Fagron	Prednicarbate, micronized	14A27-B02-295796	6
Fagron	Prednicarbate, micronized	14A27-B02-295797	6
Fagron	Prednicarbate, micronized	14A27-B02-295793	1
Fagron	Prednicarbate, micronized	701867-0001	1
Fagron	Prednicarbate, micronized	14J16B06303466	1
Fagron	Prednicarbate, micronized	14J16-B06-303465	10
Euro OTC	Prednicarbate, micronized	1501033-01	2
Caelo	Prednicarbate, micronized	14A27-B02-295796	1
Fagron	Prednicarbate, micronized	NU0823M	1
Euro OTC	Prednicarbate, micronized	1501033-02	4
Fagron	Prednicarbate, micronized	14A27-B02	1
Caelo	Prednicarbate, micronized	15181403	10
Fagron	Prednicarbate, micronized	15D15-B03-308161	5
Caelo	Prednicarbate, micronized	15D15-B03	1
Caelo	Prednicarbate, micronized	14J16-B06	3
Caelo	Prednicarbate, micronized	1507011-01	1
Fragron	Prednicarbate, micronized	NV0485M	1
Fagron	Prednicarbate, micronized	15D15-B03-308162	1
Caelo	Prednicarbate, micronized	15181409	1
Euro OTC	Prednicarbate, micronized	1507011-01	1
Caelo	Prednicarbate, micronized	15181411	2
caesar&loretz,Phönix	Prednicarbate, micronized	15181411	1
Euro	Prednicarbate, micronized	1507011-01	1
Euro OTC	Prednicarbate, micronized	1507011-02	4
Fagron	Prednicarbate, micronized	15g10-b02-310848	1
Caelo	Prednicarbate, micronized	15446301	12
Fagron	Prednicarbate, micronized	15G10-B02-314082	2
Caelo	Prednicarbate, micronized	15G10-B02-314082	3
Caelo	Prednicarbate, micronized	15181404	2
Fagron	Prednicarbate, micronized	15G10-B02-310848	5
Fagron	Prednicarbate, micronized	NU0823M	1
Fagron	Prednicarbate, micronized	15D15-B03-30816	1

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Supplier	Substance	Batch	Spectra
Fagron	Prednicarbate, micronized	15G10-B02	1
Fagron	Prednicarbate, micronized	15G10-B02-311819	1
Noweda	Prednicarbate, micronized	15446301	1
Caelo	Prednicarbate, micronized	15446302	10
Fagron	Prednicarbate, micronized	15J22-B04-316799	4
Fagron	Prednicarbate, micronized	15J22-B04-316799	1
Caelo	Prednicarbate, micronized	15446305	6
Caelo	Prednicarbate, micronized	15446303	2
Euro OTC	Prednicarbate, micronized	1601058-01	3
Caelo	Prednicarbate, micronized	15446304	1
Fagro/Gehe	Prednicarbate, micronized	15D15-B03-308161	1
Fagron	Prednicarbate, micronized	15D15-B03-309682	1
Euro OTC	Prednicarbate, micronized	1605001	1
Fagron	Prednicarbate, micronized	15J22-B04-318528	3
Fagron	Prednicarbate, micronized	15J22-B04-318930	2
Euro OTC	Prednicarbate, micronized	1605001-01	7
Caelo	Prednicarbate, micronized	15446306	5
Ebert u. Jacobi 02.0...	Prednicarbate, micronized	15446306	1
Caelo	Prednicarbate, micronized	160500	1
Fargon	Prednicarbate, micronized	15J22-B04-318930	1
Caelo	Prednicarbate, micronized	16087401	11
Caelo	Prednicarbate, micronized	1601058-01	1
Fagron	Prednicarbate, micronized	15J-B04-316799	1
Caelo	Prednicarbate, micronized	16087408	13
AHL	Prednicarbate, micronized	16087408	2
Fagron	Prednicarbate, micronized	160518P	1
Fagron	Prednicarbate, micronized	160314PC	1
Bombastus	Prednicarbate, micronized	15446306	1
Fagron	Prednicarbate, micronized	16A18/B01	1
Sonnenberg-Apotheke	Prednicarbate, micronized	1607012-01	1
Celo	Prednicarbate, micronized	1687408	1
Caelo	Prednicarbate, micronized	15J22-B-321005	1
Caelo	Prednicarbate, micronized	1607012-01	2
Euro OTC	Prednicarbate, micronized	1607012-01	5
Caelo	Prednicarbate, micronized	16A18-B01-322732	1
Caelo	Prednicarbate, micronized	16087410	12
Caelo	Prednicarbate, micronized	16987410	1
Caelo	Prednicarbate, micronized	1608710	1
Caelo/Sanacorp	Prednicarbate, micronized	15546306	1
Caelo	Prednicarbate, micronized	16A18-B01-322733	2
caesar&loretz GmbH,AHC,...	Prednicarbate, micronized	16087408	1
Fagron	Prednicarbate, micronized	16A18-B01-322732	3
Caelo	Prednicarbate, micronized	16087412	5
Fagron	Prednicarbate, micronized	16E12-B01	2
Fagron	Prednicarbate, micronized	16E12-B01-325758	3
Caelo	Prednicarbate, micronized	16087411	3
Euro OTC	Prednicarbate, micronized	1609022-01	15
Caelo	Prednicarbate, micronized	1609022-01	3
Sanacorp, 01.03.17, 21,...	Prednicarbate, micronized	1687410	1
Caesar & Loretz GmbH	Prednicarbate, micronized	16087410	1
Fagron	Prednicarbate, micronized	16E12-B01-328270	3
Fagron	Prednicarbate, micronized	16E12-B01-327344	3
Caelo	Prednicarbate, micronized	17013804	10
Caelo	Prednicarbate, micronized	17013805	5
Caelo	Prednicarbate, micronized	1517E-03595	1
Fagron	Prednicarbate, micronized	17013804	1
Noweda/Apomix	Prednicarbate, micronized	1609022-01	2
Noweda	Prednicarbate, micronized	17013804	2
Phönix	Prednicarbate, micronized	16J27-B01-330976	1
Phönix	Prednicarbate, micronized	15J22-B04-318528	1

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Supplier	Substance	Batch	Spectra
Caelo	Prednicarbate, micronized	17014003	12
Fagron	Prednicarbate, micronized	16J27-b01-330976	1
Fagron	Prednicarbate, micronized	16E12-B01-330093	1
Fagron	Prednicarbate, micronized	16J27-B01-330976	4
Fagron	Prednicarbate, micronized	160902201	1
Caelo	Prednicarbate, micronized	16E12-B01-325758	1
Caelo	Prednicarbate, micronized	15J22-B04-318528	1
Fagron	Prednicarbate, micronized	16J28-B01-330976	1
Fagron	Prednicarbate, micronized	1612-B01-325758	1
Phoenix	Prednicarbate, micronized	16J27-b01-332958	1
Caelo	Prednicarbate, micronized	17014001	2
Hedinger	Prednicarbate, micronized	16J27-B01-330976	2
Kehr	Prednicarbate, micronized	16J27-B01-330976	1
Fagron	Prednicarbate, micronized		1
Fagron	Prednicarbate, micronized	16/27-B01-332958	2
Fagron	Prednicarbate, micronized	16J27-B01-332958	3
Euro OTC	Prednicarbate, micronized	160902	1
Caelo	Prednicarbate, micronized	17014005	7
Newchem Spa/Sanacorp	Prednicarbate, micronized	16E12-B01	1
Fagron	Prednicarbate, micronized	16j27-b01-330976	1
Euro OTC	Prednicarbate, micronized	1707022-01	11
Fagron	Prednicarbate, micronized	16j27b01330976	1
Caelo	Prednicarbate, micronized	17220407	14
Fagron	Prednicarbate, micronized	17C27-B01-335530	7
Fagron	Prednicarbate, micronized	16J27-B01-330977	1
Fagron	Prednicarbate, micronized	17C27-B01-335531	1
Caelo	Prednicarbate, micronized	17220408	16
Caelo	Prednicarbate, micronized	17220401	1
Fagron	Prednicarbate, micronized	17c27-b01-339079	1
Fagron	Prednicarbate, micronized	17C27-B01-339079	1
Caelo	Prednicarbate, micronized	17014006	1
Caelo	Prednicarbate, micronized	17220406	1
Bombastus	Prednicarbate, micronized	17220408	1
Caelo	Prednicarbate, micronized	172204075515	1
Fagron	Prednicarbate, micronized	17J04-B05-340570	1
Euro OTC	Prednicarbate, micronized	1801013-01	4
Caelo	Prednicarbate, micronized	17C27-B01-339079	1
Caelo	Prednicarbate, micronized	1707022-01	2
Caelo	Prednicarbate, micronized	17220410	1
Caelo	Prednicarbate, micronized	17315603	1
Sanacorp	Prednicarbate, micronized	17315604	1
Caelo	Prednicarbate, micronized	17315604	10
Caelo	Prednicarbate, micronized	1801013-01	4
Fagron	Prednicarbate, micronized	174J04-B05-343935	1
Anzag	Prednicarbate, micronized	17220408	1
Euro OTC	Prednicarbate, micronized		1
Fagron	Prednicarbate, micronized	17J04-B05-341872	3
Caelo	Prednicarbate, micronized		2
Fagron	Prednicarbate, micronized	NX1422M	1
Hepart	Prednicarbate, micronized	17C27-B01-335530	1
Caelo	Prednicarbate, micronized	17315605	6
Caelo	Prednicarbate, micronized	17315607	1
Euro OTC	Prednicarbate, micronized	180101301	1
Fagron	Prednicarbate, micronized	17J04-B05-346113	4
Fagron	Prednicarbate, micronized	17J04-B05-326113	1
AHD	Prednicarbate, micronized	1801013-01	1
Fagron	Prednicarbate, micronized	18B27-B01-0001	1
Caelo	Prednicarbate, micronized	17315609	5
Cealo/GEHE	Prednicarbate, micronized	17315609	1
Caelo	Prednicarbate, micronized	17J04-B05-346113	1

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Supplier	Substance	Batch	Spectra
Jenne	Prednicarbate, micronized	17J04-B05-346113	1
Euro OTC	Prednicarbate, micronized	1805005-01	4
Fagron	Prednicarbate, micronized	18B27-B01-350264	3
Euro OTC	Prednicarbate, micronized	1801013	1
Fagron	Prednicarbate, micronized	18B27-B01-347486	1
Fagron	Prednicarbate, micronized	18B27-01-347486	1
Fagron	Prednicarbate, micronized	18194104	1
Euro OTC	Prednicarbate, micronized	1809015-01	3
Caelo	Prednicarbate, micronized	18194104	6
Fagron	Prednicarbate, micronized	18B27-01-350264	1
Caelo	Prednicarbate, micronized	18194105	6
Fagron	Prednicarbate, micronized	18E14-B03-352631	1
Fagron	Prednicarbate, micronized	18E14B03-352560	1
Fagron	Prednicarbate, micronized	18E14-B03	1

- 78 368 spectra from 565 *Apo-Ident* customers from a total of 25 978 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Prednicarbate, micronized* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednicarbate, micronized* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	506	0	73 990
Type B	0	870	0	126 022
Type C	0	547	14	78 368

The substance/substance group *Prednicarbate, micronized* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.8142 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 99.3103 %)
Type C	100.0000 % (> 99.8817 %)	97.5045 % (> 96.9697 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21572	21572	0.00	40.62
20700	21572	10.36	44.86
21368	21368	0.00	32.59
21369	21368	1.58	32.90
21610	21610	0.00	29.54
21858	21858	0.00	31.51
20832	20832	0.00	39.65
20833	20832	2.08	39.49
22366	22366	0.00	32.56

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Prednisolon dihydrogen phosphate dinatrium**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20212-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Prednisolon dihydrogen phosphate dinatrium; Prednisoloni natrii phosphas

Special notes

When selecting the *Prednisolon dihydrogen phosphate dinatrium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Prednisolon dihydrogen phosphate dinatrium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisolon dihy...	13304703	20923	40	20130904
Caelo	Prednisolon dihy...	13304704	21412	40	1411052
Fagron	Prednisolon dihy...	14E07-B06-295251	21571	40	20140623
Fagron	Prednisolon dihy...	18D23-B08-351348	24293	40	1812421

Validation samples

A total of 280317 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 *Prednisolon dihydrogen phosphate dinatrium*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 *Prednisolon dihydrogen phosphate dinatrium*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednisolon dihydrogen phosph...	13304704	21412 [†]	20
Caelo	Prednisolon dihydrogen phosph...	13304704	21413	60
Fagron	Prednisolon dihydrogen phosph...	14E07-B06-295251	21571 [†]	20
Fagron	Prednisolon dihydrogen phosph...	16I14-B03-328918	23270	40
Caelo	Prednisolon dihydrogen phosph...	16174715	23271	40

- 126712 spectra from a total of 2785 batches from further 781 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 33 *Apo-Ident* customers from 44 batches from the substance/substance group *Prednisolon dihydrogen phosphate dinatrium*.

[†]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
Fagron	Prednisolon dihydrogen phosp...	12H30-N08	2
Fagron	Prednisolon dihydrogen phosp...	11C18-N11	1
Fagron	Prednisolon dihydrogen phosp...	13A10-N04	3
Fagron	Prednisolon dihydrogen phosp...	11K11-N11	2
Fagron	Prednisolon dihydrogen phosp...	13C26N06	1
Fagron	Prednisolon dihydrogen phosp...	13I27-N01	3
Fagron	Prednisolon dihydrogen phosp...	13H19N04	1
Fagron	Prednisolon dihydrogen phosp...	13/27-N01	1
Caelo	Prednisolon dihydrogen phosp...	14196602	1
Fagron	Prednisolon dihydrogen phosp...	14E07-B06-295251	3
Fagron	Prednisolon dihydrogen phosp...	14G30-B09-303012	6
Fagron	Prednisolon dihydrogen phosp...	14E07-B06-295253	1
Fagron	Prednisolon dihydrogen phosp...	14G30-B09-303014	4
Fagron	Prednisolon dihydrogen phosp...	14G30-B09	1
Fagron	Prednisolon dihydrogen phosp...	NU1356	1
Caelo	Prednisolon dihydrogen phosp...	15199602	2
Fagron	Prednisolon dihydrogen phosp...	15f29-b11-309694	1
Fagron	Prednisolon dihydrogen phosp...	15F29-B11-309694	1
Fagron	Prednisolon dihydrogen phosp...	14g30-b09-303014	1
Fagron	Prednisolon dihydrogen phosp...	15J01-B02-313610	2
Fagron	Prednisolon dihydrogen phosp...	15J01-B02-312722	3
Caelo	Prednisolon dihydrogen phosp...	15199603	1
Newchem spa	Prednisolon dihydrogen phosp...	15J01-B02-313610	2
Fagron	Prednisolon dihydrogen phosp...	15J01-B02	4
Fagron	Prednisolon dihydrogen phosp...	15J01-B02-317180	2
Fagron	Prednisolon dihydrogen phosp...	15K27-B09-318738	2
Alte Apotheke	Prednisolon dihydrogen phosp...	15K27B09-318738	1
Fagron	Prednisolon dihydrogen phosp...	15K27-B09-322162	1
Fagron	Prednisolon dihydrogen phosp...	15K27-B09	3
Caelo	Prednisolon dihydrogen phosp...	16174702	1
Caelo	Prednisolon dihydrogen phosp...	16174701	1
Fagron	Prednisolon dihydrogen phosp...	15K27-B09-326263	3
Fagron	Prednisolon dihydrogen phosp...	15K27B09-326263	1
Caelo	Prednisolon dihydrogen phosp...	16174710	1
Caelo	Prednisolon dihydrogen phosp...	16174706	1
Fagron	Prednisolon dihydrogen phosp...	16I14-B03-328918	2
Fagron	Prednisolon dihydrogen phosp...	16/14-B03-328169	1
Caelo	Prednisolon dihydrogen phosp...	17077502	1
Fagron	Prednisolon dihydrogen phosp...	15k27-b09-318738	1
Fagron	Prednisolon dihydrogen phosp...	16I14-B03	1
Fagron	Prednisolon dihydrogen phosp...	17/27-b03-342560	1
Sidonia	Prednisolon dihydrogen phosp...	17I27-B03-344246	1
Sidonia	Prednisolon dihydrogen phosp...	17I27-B03-345405	6
Sidonia	Prednisolon dihydrogen phosp...	17I27-B03-342560	1
Caelo	Prednisolon dihydrogen phosp...	18024602	1

- 78 848 spectra from 565 *Apo-Ident* customers from a total of 26 094 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Prednisolon dihydrogen phosphate dinatrium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with

Prednisolon dihydrogen phosphate dinatrium and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	157	3	74 336
Type B	0	180	0	126 712
Type C	0	80	1	78 848

The substance/substance group *Prednisolon dihydrogen phosphate dinatrium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	98.1250 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	98.7654 % (> 95.0617 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20923	21412	11.30	40.18
21412	21412	0.00	33.95
21571	21412	13.10	47.54
24293	24293	0.00	20.21

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Prednisolone acetate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20089-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednisolone acetate; Prednisoloni acetas

Special notes

When selecting the *Prednisolone acetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Prednisolone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisolone ace...	12091814	20784	80	20120416
Fagron	Prednisolone ace...	12H14-N07	20795	40	20120829
Caelo	Prednisolone ace...	12324502	20877	40	20121112
Euro OTC	Prednisolone ace...	1306040	21096	40	20130812
Caelo	Prednisolone ace...	13262605	21450	40	20130923

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prednisolone ace...	1209028-03	21530	40	AR-15-FG-010480-01
Euro OTC	Prednisolone ace...	1512020	22297	30	20160119*
Fagron	Prednisolone ace...	12H14-N07	20795SI	34	20120829
Caelo	Prednisolone ace...	13262605	21450SI	36	20130923
Euro OTC	Prednisolone ace...	1512020	22297SI	29	20160119*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 409 spectra of 10 reference samples from the substance/substance group *Prednisolone acetate*. These samples are listed above in the [calibration samples](#) section.
- 74 087 spectra from a total of 1616 batches from further 372 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 [†].

- 424 spectra of 14 reference samples from the substance/substance group *Prednisolone acetate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednisolone acetate	13262605	21448	60
Caelo	Prednisolone acetate	13262605	21450 [†]	20
Euro OTC	Prednisolone acetate	1209028-03	21530 [†]	20
Euro OTC	Prednisolone acetate	1512020	22297 [†]	15
Euro OTC	Prednisolone acetate	1607010	22710	40
Euro OTC	Prednisolone acetate	1701041	23142	40
Euro OTC	Prednisolone acetate	1805009	24133	40
Fagron	Prednisolone acetate	12H14-N07	20795SI [†]	15
Caelo	Prednisolone acetate	13262605	21448SI	44
Caelo	Prednisolone acetate	13262605	21450SI [†]	11
Euro OTC	Prednisolone acetate	1512020	22297SI [†]	15
Euro OTC	Prednisolone acetate	1607010	22710SI	40
Euro OTC	Prednisolone acetate	1701041	23142SI	24
Euro OTC	Prednisolone acetate	1805009	24133SI	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.

- 126 468 spectra from a total of 2782 batches from further 781 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.

- 1084 spectra from 365 *Apo-Ident* customers from 218 batches from the substance/substance group *Prednisolone acetate*.

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone acetate	11158002	1
Euro OTC	Prednisolone acetate	1108043-01	2
Euro OTC	Prednisolone acetate	1108043-02	10
Fagron	Prednisolone acetate	12C19-N03	4
Caelo	Prednisolone acetate	11158003	1
Euro OTC	Prednisolone acetate	2507212106	1
Caelo	Prednisolone acetate	12091802	6
Fagron	Prednisolone acetate	12C19-N03	1
Fagron	Prednisolone acetate	11I09N-08	1
Fagron	Prednisolone acetate	11I09-N08	1
Fagron	Prednisolone acetate	12G25-N05	5
Caelo	Prednisolone acetate	12091803	3
Caelo	Prednisolone acetate	12091804	8
Euro OTC	Prednisolone acetate	711212106	1
Fagron	Prednisolone acetate	12H14-N07	4
Gehe	Prednisolone acetate	12H14-N07	1
Fagron	Prednisolone acetate	11A31-N03	1
ANZAG	Prednisolone acetate	12091802	2
Fargo	Prednisolone acetate	12025-N05	1
Fagron	Prednisolone acetate	113Q-02106	1
Caelo	Prednisolone acetate	12091807	5
Caelo	Prednisolone acetate	12091808	4
Euro OTC	Prednisolone acetate	1209028-01	3
Caelo	Prednisolone acetate	6021306	1
Caelo	Prednisolone acetate	11L21-N03	1
Fagron	Prednisolone acetate	12J10-N05	1
Caelo	Prednisolone acetate	12091814	7
Noweda	Prednisolone acetate	1209028-01	1
Fagron	Prednisolone acetate	12L05-N01	5
Caelo	Prednisolone acetate	12091806	3
Sanacorp	Prednisolone acetate	12091808	1
Caelo	Prednisolone acetate	12091813	1
Caelo	Prednisolone acetate	12091815	2
Caelo	Prednisolone acetate	12324502	11
Euro OTC	Prednisolone acetate	1209028-02	11
Phönix	Prednisolone acetate	11158008	1
Caelo	Prednisolone acetate	12091810	2
Caelo	Prednisolone acetate		2
Gehe	Prednisolone acetate	1209028-02	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
Euro OTC	Prednisolone acetate	200540	2
Alliance Healthcare	Prednisolone acetate	12091807	1
Caelo	Prednisolone acetate	12324504	6
Fagron	Prednisolone acetate	12324502	1
Fagron	Prednisolone acetate	13a07n07	1
Fagron	Prednisolone acetate	13A07-N07	6
Anzag	Prednisolone acetate	13A07N07	1
Gehe	Prednisolone acetate	1209028-01	1
Euro OTC	Prednisolone acetate	2413Q02106	1
A.H. 23.05.13 ek: 5,40EUR	Prednisolone acetate	13A07-N07	1
Caelo	Prednisolone acetate	1209028-02	2
Caelo	Prednisolone acetate	12324505	16
Alliance	Prednisolone acetate	1209028-02	2
Caelo	Prednisolone acetate	11080403	1
Fagron	Prednisolone acetate	180713a	1
Phönix	Prednisolone acetate	1209028-02	1
Fagron	Prednisolone acetate	6082013D	1
Caelo	Prednisolone acetate	12324506	11
Fagron	Prednisolone acetate	12J10/N05	1
Caelo	Prednisolone acetate	12L05-N01	1
Phönix	Prednisolone acetate	12324506	1
Euro OTC	Prednisolone acetate	1306040-01	20
Caelo	Prednisolone acetate	12324508	9
Caelo	Prednisolone acetate	4313A-02106	1
Noweda	Prednisolone acetate	12324506	1
Caelo	Prednisolone acetate	1234506	1
Fargon	Prednisolone acetate	13A07-N07	1
Symbiotika/Anzag	Prednisolone acetate	1306040-01	1
Fagron	Prednisolone acetate	13D03-N06	1
EUro/AHD	Prednisolone acetate	1306040-01	1
Fagron	Prednisolone acetate	12L11-B40-286905	12
Caelo	Prednisolone acetate	12324509	2
Caelo	Prednisolone acetate	13262601	14
Euro OTC	Prednisolone acetate	1209028	1
Caelo	Prednisolone acetate	13262602	7
Caelo	Prednisolone acetate	27051301	1
Caelo	Prednisolone acetate	1306040-01	1
Euro OTC	Prednisolone acetate	514U2106	1
Fagron	Prednisolone acetate	12L11-B40	1
EUro/AHD	Prednisolone acetate	1306040-02	1
Caelo	Prednisolone acetate	13262603	8
Fagron	Prednisolone acetate	12L11-B40-286915	2
Euro OTC	Prednisolone acetate	1306040-02	14
Euro OTC	Prednisolone acetate	1306040-1	1
Symbiotica Spec./Phönix	Prednisolone acetate	1306040-02	1
Caelo	Prednisolone acetate	13262605	10
Euro OTC	Prednisolone acetate	130604002	1
VDL;7,15EUR, 21:06:14	Prednisolone acetate	13262602	1
Euro OTC	Prednisolone acetate	5012I-02106	1
Caelo	Prednisolone acetate	13262606	2
Fagron	Prednisolone acetate	200540-0013	1
Fagron	Prednisolone acetate	13262605	1
GEHE 03.07.2014	Prednisolone acetate	13262605	1
Euro OTC	Prednisolone acetate	1209028-03	2
EuRho	Prednisolone acetate	1306040-03	1
Caelo	Prednisolone acetate	12324514	5
Fagron	Prednisolone acetate	13K20-B04-289495	3
Caelo	Prednisolone acetate	313I-02106	1
Fagron	Prednisolone acetate	12L11-B04-286905	1
Caesar&loretz,Phoenix	Prednisolone acetate	13262606	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Prednisolone acetate	1203028-03	1
Euro OTC	Prednisolone acetate	1406014-01	15
Euro OTC	Prednisolone acetate	13262606	1
Fagron	Prednisolone acetate	13K20-B04-289494	2
Euro OTC	Prednisolone acetate	1306040-03	1
Phoenix	Prednisolone acetate	12L11-B40-286905	1
Fagron	Prednisolone acetate	12k20-b04293971	1
Gehe	Prednisolone acetate	1406014-01	1
Caelo	Prednisolone acetate	1406014-01	2
Lihua Pharma	Prednisolone acetate	1406014-01	1
Caelo	Prednisolone acetate	1406014-02	2
Caelo	Prednisolone acetate	14175513	10
noweda	Prednisolone acetate	14175513	1
Gehe	Prednisolone acetate	13262609	1
Euro OTC	Prednisolone acetate	1406014-02	11
Kehr	Prednisolone acetate	1406014-01	1
Caelo	Prednisolone acetate	12324503	1
Fagron	Prednisolone acetate	13K20-B04-293971	2
AHD 23.10.14 EK17,24	Prednisolone acetate	13262601	1
Caelo	Prednisolone acetate	14175508	13
Caelo	Prednisolone acetate	13262609	2
Cealo	Prednisolone acetate	14175513	1
Caelo	Prednisolone acetate	14175514	6
Fagron	Prednisolone acetate	14D04-B03-299294	4
Euro OTC	Prednisolone acetate	1406012-02	1
Fagron	Prednisolone acetate	13K20-B04-293970	1
Euro OTC	Prednisolone acetate	289295	1
AHD 06.03.15	Prednisolone acetate	14175508	1
Caesar&loretz,Phoenix	Prednisolone acetate	14175513	1
Noweda	Prednisolone acetate	12L11-B40-286905	1
Euro OTC	Prednisolone acetate	150103601	3
Euro OTC	Prednisolone acetate	1501036-01	18
Phönix	Prednisolone acetate	13262605	2
Caelo	Prednisolone acetate	14175509	8
Fagron	Prednisolone acetate	14G30-B13	1
Caelo	Prednisolone acetate	15055201	7
Euro OTC	Prednisolone acetate	2714U-02106	1
Caelo	Prednisolone acetate	15055203	2
Lihua Pharm	Prednisolone acetate	K07A20140302M	1
Fagron	Prednisolone acetate	14G30-B13-302562	1
Noweda 18.05.2015	Prednisolone acetate	14D04-B03-299294	1
Euro OTC	Prednisolone acetate	1460614-01	1
Caelo	Prednisolone acetate	14380901	14
A.H.D.	Prednisolone acetate	14175514	1
Caelo	Prednisolone acetate	15055202	14
Fagron	Prednisolone acetate	14G30-B13-299293	2
Fagron	Prednisolone acetate	14D04B03299295	1
Noweda	Prednisolone acetate	15055202	1
Caelo	Prednisolone acetate	14175512	1
caesar&loretz,Phönix	Prednisolone acetate	15055202	2
Fagron	Prednisolone acetate	K07A20130903M	1
Euro OTC	Prednisolone acetate	1501036-02	27
Fagron	Prednisolone acetate	15B03-B05-308582	3
Caelo	Prednisolone acetate	14380902	10
Euro OTC	Prednisolone acetate	1501036	1
Euro OTC	Prednisolone acetate	K07A20140304M	1
Caelo	Prednisolone acetate	1475509	1
AllianceHealthcare	Prednisolone acetate	15055201	1
Caelo	Prednisolone acetate	14380302	1
Caelo	Prednisolone acetate	15055206	8

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Supplier	Substance	Batch	Spectra
Fragron	Prednisolone acetate	K07A20131101M	1
Caelo	Prednisolone acetate	1480905	1
Caelo	Prednisolone acetate	14380904	2
Euro OTC	Prednisolone acetate		2
Caelo	Prednisolone acetate	14380909	11
Caelo	Prednisolone acetate	14380905	15
Sanacorp	Prednisolone acetate	15055206	1
Henan Lihua Pharmaceuti...	Prednisolone acetate	14G30-B13	1
Euroo/Gehe	Prednisolone acetate	1501036-02	1
sanacorp	Prednisolone acetate	14380909	1
caesar&loretz	Prednisolone acetate	14380909	1
Euro OTC	Prednisolone acetate	1512020-01	25
EuRho	Prednisolone acetate	1512020-01	1
Cael Sanacorp 05.02.2016	Prednisolone acetate	14380901	1
Cael Sanacorp 05.02.2016	Prednisolone acetate	14175509	1
Caelo	Prednisolone acetate	14380910	11
Caesar/Loretz,Fa.Gehe	Prednisolone acetate	14380910	1
phönix	Prednisolone acetate	1512020-01	1
apo-ident	Prednisolone acetate	1512020-01	1
Caelo	Prednisolone acetate	1616I-02106	1
Caelo	Prednisolone acetate	15398302	11
Fagron	Prednisolone acetate	15B03-B05-302566	1
Caelo	Prednisolone acetate	1512020-01	3
Beiersdorf AG	Prednisolone acetate	15398302	1
Beiersdorf AG	Prednisolone acetate	15055201	1
Caelo	Prednisolone acetate	15398304	6
phönix	Prednisolone acetate	14380902	2
Caelo	Prednisolone acetate	15398303	10
	Prednisolone acetate	15398303	1
Fagron	Prednisolone acetate	15803-B05	1
Caesar&Loretz,Phönix,08...	Prednisolone acetate	15398302	1
Euro OTC	Prednisolone acetate	151202001	1
Caelo	Prednisolone acetate	15398307	9
Caesar&loretz,Phoenix,2...	Prednisolone acetate		1
Euro OTC	Prednisolone acetate	2215I-02106	1
Wolf-Apotheke	Prednisolone acetate	14380911	1
Caelo	Prednisolone acetate	20160727Ma1	1
Sanacorp	Prednisolone acetate	15398408	1
phönix	Prednisolone acetate	14380910	1
Fagron	Prednisolone acetate	15B03-B05-302564	10
Noweda	Prednisolone acetate	15398303	1
phönix	Prednisolone acetate	15398303	1
Caelo	Prednisolone acetate	15398306	3
Caelo	Prednisolone acetate	15398401	7
Caesar&loretz,AHC,29.08...	Prednisolone acetate	15398306	1
Caelo	Prednisolone acetate	15398408	9
Euro OTC	Prednisolone acetate	1607010-01	68
Fagron	Prednisolone acetate	15b03-b05-302564	1
Caesar&Loretz GmbH	Prednisolone acetate	15396408	1
Fagron	Prednisolone acetate	115B03-B05-308582	1
Caelo	Prednisolone acetate	15398402	9
Euro OTC	Prednisolone acetate	161005PA	1
Caelo	Prednisolone acetate	15398407	8
Bombastus	Prednisolone acetate	2255	1
phönix	Prednisolone acetate	15398402	1
Fagron	Prednisolone acetate	15398401	1
Caelo	Prednisolone acetate	1607010-01	4
phönix	Prednisolone acetate	1438910	1
Phoenix	Prednisolone acetate	14380905	1
Caelo	Prednisolone acetate	16246801	10

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Supplier	Substance	Batch	Spectra
Euro OTC	Prednisolone acetate	150103602	1
Caelo	Prednisolone acetate	1624801	1
Caelo	Prednisolone acetate	16246804	8
Caelo	Prednisolone acetate	16246802	7
Euro OTC	Prednisolone acetate	16246801	2
Phönix	Prednisolone acetate	16246804	1
Caelo	Prednisolone acetate	15396304	1
Caelo	Prednisolone acetate	16246803	10
Caelo	Prednisolone acetate	160701001	2
Caelo	Prednisolone acetate	14380903	2
phönix	Prednisolone acetate	16246803	3
Euro OTC	Prednisolone acetate	1607010-10	1
Caelo	Prednisolone acetate	717Q-02106	1
PhönixWE:10.02.2017 E...	Prednisolone acetate	16246806	1
Caelo	Prednisolone acetate	151202001	1
Caelo	Prednisolone acetate	165246802	1
Caesar&LoretzGmbH,11,03...	Prednisolone acetate	16246803	1
Caelo	Prednisolone acetate	16246805	1
Caelo	Prednisolone acetate	162468	2
Caelo	Prednisolone acetate	16246806	8
Caelo	Prednisolone acetate	16246807	8
Gehe	Prednisolone acetate	16246806	2
Caelo	Prednisolone acetate	1624806	1
Gehe	Prednisolone acetate	16246803	2
phönix	Prednisolone acetate	16246806	1
Caelo	Prednisolone acetate	16246808	9
Euro OTC	Prednisolone acetate	170413PA/1607010-01	1
Phönix	Prednisolone acetate	15398303	1
Noweda	Prednisolone acetate	K07D20150105M	1
Euro OTC	Prednisolone acetate	160701001	1
Fagron	Prednisolone acetate	K07D20150105M	2
GEHE	Prednisolone acetate	16246807	1
Caelo	Prednisolone acetate	16246809	1
Fagron	Prednisolone acetate	15123-B04-327929	1
Caelo	Prednisolone acetate	16246811	4
Euro OTC	Prednisolone acetate	1701041-01	14
Fagron	Prednisolone acetate	15F29-B07-323268	1
Caelo	Prednisolone acetate	17086103	9
Caesar&Loretz GmbH,PHön...	Prednisolone acetate	17086103	2
Anzag	Prednisolone acetate	16246812	1
Caelo	Prednisolone acetate	16246812	3
Fagron	Prednisolone acetate	15B03-B05	1
Caelo	Prednisolone acetate	17086102	5
Finteler Apotheke	Prednisolone acetate	16246812	1
Caelo	Prednisolone acetate	16248808	1
Delta	Prednisolone acetate	17086103	1
phönix	Prednisolone acetate	16246807	1
Finteler Apotheke	Prednisolone acetate	17086103	1
Fagron	Prednisolone acetate	5444	1
Caesar & Loretz GmbH, P...	Prednisolone acetate	17185601	1
Euro OTC	Prednisolone acetate	170104101	1
Euro OTC	Prednisolone acetate	K07D20161003M	1
Caelo	Prednisolone acetate	17185603	9
Caelo	Prednisolone acetate	17086105	6
Caelo	Prednisolone acetate	17086104	10
Noweda	Prednisolone acetate	1523-B04-334688	1
Caelo	Prednisolone acetate	17086106	2
Noweda/EuRo	Prednisolone acetate	1607010-01	1
Fagron	Prednisolone acetate	1523-B04	1
Phönix	Prednisolone acetate	17185602	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Prednisolone acetate	17086104	1
Caelo	Prednisolone acetate	17086101	5
Caelo	Prednisolone acetate	17185601	9
Caelo	Prednisolone acetate	17086103/1110917	1
Sanacorp	Prednisolone acetate	17185601	1
Caelo	Prednisolone acetate	162446808	1
GEHE	Prednisolone acetate	17185601	1
Euro OTC	Prednisolone acetate	1701041-02	9
Fagron	Prednisolone acetate		1
Caelo	Prednisolone acetate	1701041-02	2
Fagron	Prednisolone acetate	15123-B04-331154	2
Eurho	Prednisolone acetate	1701041-01	2
Euro OTC	Prednisolone acetate	170104102	1
Caelo	Prednisolone acetate	170861015494	1
Sanacorp	Prednisolone acetate	15123-B04-341793	1
Bombastus	Prednisolone acetate	17185601	1
Caelo	Prednisolone acetate	171856010	1
Phönix W.E:17.03.18 E...	Prednisolone acetate	17185601	1
Caelo	Prednisolone acetate	17185602	6
Sanacorp	Prednisolone acetate	17185602	1
Delta	Prednisolone acetate	17185602	1
Euro OTC	Prednisolone acetate	1701041-03	2
Gehe/EuRo	Prednisolone acetate	1701041-02	1
Fagron	Prednisolone acetate	12h14-n07	1
Caelo	Prednisolone acetate	18004401	6
Noweda	Prednisolone acetate	17010410203707556	1
Fagron	Prednisolone acetate	15123-B4-334688	1
Caelo	Prednisolone acetate	17185604	2
EuRho/Noweda	Prednisolone acetate	18004401	1
Euro OTC	Prednisolone acetate	1805009-01	10
Caelo	Prednisolone acetate	18067301	2
Euro OTC	Prednisolone acetate	18004403	1
EuRho	Prednisolone acetate	170104102	1
Sanacorp	Prednisolone acetate	15123-B04-334688	2
Caelo	Prednisolone acetate	18004403	1
Caelo	Prednisolone acetate	18004402	1
Caelo	Prednisolone acetate	180673025724	1
Fagron	Prednisolone acetate	1805009-01	1
Sanacorp	Prednisolone acetate	18067303	2
EuRho	Prednisolone acetate	1406014-02	1
Fagron	Prednisolone acetate	15/23-B04-334702	1
Caelo	Prednisolone acetate	18067309	6
Caelo	Prednisolone acetate	18067302	2
Euro OTC	Prednisolone acetate	18067302	1
Caelo	Prednisolone acetate	18398303	1
Caelo	Prednisolone acetate	18067307	2
Euro OTC	Prednisolone acetate	1805009-02	3
Caelo	Prednisolone acetate	18067309-P20180115Ma	1
Caelo	Prednisolone acetate	18067303	2

- 77 845 spectra from 565 *Apo-Ident* customers from a total of 25 925 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Prednisolone 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 *Prednisolone 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	409	0	74 087
Type B	0	424	0	126 468
Type C	0	1042	42	77 845

The substance/substance group *Prednisolone 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 % (> 99.9887 %)	100.0000 % (> 98.5330 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.5849 %)
Type C	100.0000 % (> 99.8817 %)	96.1255 % (> 95.8487 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20784	21530	6.74	45.84
20877	21530	4.82	44.60
21530	21530	0.00	41.57
22297	22297	0.00	41.51
21096	21530	3.83	43.25
21450	22297	6.96	39.37
20795	22297	5.48	42.52

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Prednisolone hydrogen succinate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20838-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednisolone hydrogen succinate; Prednisoloni hydrogenosuccinas

Special notes

When selecting the *Prednisolone hydrogen succinate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Prednisolone hydrogen succinate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Prednisolone hyd...	13D16-N11	20956	40	1509250
Fagron	Prednisolone hyd...	14G29-B07-304733	22652	40	1701370

Validation samples

A total of 280317 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 *Prednisolone hydrogen succinate*. These samples are listed above in the [calibration samples](#) section.
- 74416 spectra from a total of 1621 batches from further 372 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 *Prednisolone hydrogen succinate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Prednisolone hydrogen succin...	12A20-N11	20838	40
Fagron	Prednisolone hydrogen succin...	14G29-B07-304733	22723	40
Fagron	Prednisolone hydrogen succin...	15C11-B05-344778	24058	40

- 126772 spectra from a total of 2786 batches from further 781 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 6 *Apo-Ident* customers from 8 batches from the substance/substance group *Prednisolone hydrogen succinate*.

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone hydrogen succin...	12A20-N11	1
Caelo	Prednisolone hydrogen succin...	15C11-B05-305533	1
Phönix	Prednisolone hydrogen succin...	13H24-N04	1
Caelo	Prednisolone hydrogen succin...	19081502	1

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Supplier	Substance	Batch	Spectra
Fagron	Prednisolone hydrogen succin...	14G29-B07-304733	1
Caelo	Prednisolone hydrogen succin...	15C11B05328275	1
Fagron	Prednisolone hydrogen succin...	15C11-B05-338297	1
Fagron	Prednisolone hydrogen succin...	15c11-B05338297	1

- 78 921 spectra from 565 *Apo-Ident* customers from a total of 26 129 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Prednisolone hydrogen succinate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisolone hydrogen succinate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	120	0	126 772
Type C	0	8	0	78 921

The substance/substance group *Prednisolone hydrogen succinate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8818 %)	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
20956	20956	0.00	41.29
22652	22652	0.00	42.14

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Prednisolone, micronized**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20773-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Prednisolone, micronized; Prednisolonum micronisatum

Special notes

When selecting the *Prednisolone, micronized* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Prednisolone, micronized*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisolone, mi...	12324202	20773	40	20121113
Caelo	Prednisolone, mi...	12324226	21303	39	1411271
Caelo	Prednisolone, mi...	13343105	21449	40	1411232
Euro OTC	Prednisolone, mi...	1212021-02	21604	40	1411270
Fagron	Prednisolone, mi...	13H07-B02-285592	21660	40	20130909

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prednisolone, mi...	1501047-01	21849	40	AR-15-FG-015509-01
Caelo	Prednisolone, mi...	154000	22435	40	20160225*
Caelo	Prednisolone, mi...	161343	22467	40	20160601*
Fagron	Prednisolone, mi...	14I10-B03-302263	22651	40	20141020
Euro OTC	Prednisolone, mi...	1607011	22709	40	20160818*
Caelo	Prednisolone, mi...	15400002	22783	40	20160225
Fagron	Prednisolone, mi...	16C15-B01-320761	22803	40	20160407
Euro OTC	Prednisolone, mi...	1212021-02	21604SI	33	1411270
Fagron	Prednisolone, mi...	13H07-B02-285592	21660SI	40	20130909
Euro OTC	Prednisolone, mi...	1501047-01	21849SI	20	AR-15-FG-015509-01
Caelo	Prednisolone, mi...	154000	22435SI	39	20160225*
Caelo	Prednisolone, mi...	161343	22467SI	31	20160601*
Fagron	Prednisolone, mi...	14I10-B03-302263	22651SI	40	20141020
Euro OTC	Prednisolone, mi...	1607011	22709SI	40	20160818*
Caelo	Prednisolone, mi...	15400002	22783SI	40	20160225
Fagron	Prednisolone, mi...	16C15-B01-320761	22803SI	36	20160407

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 798 spectra of 21 reference samples from the substance/substance group *Prednisolone, micronized*. These samples are listed above in the [calibration samples](#) section.
- 73 698 spectra from a total of 1611 batches from further 372 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 [†].

- 500 spectra of 19 reference samples from the substance/substance group *Prednisolone, micronized*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Prednisolone, micronized	1108055-04	20855	40
Caelo	Prednisolone, micronized	13343105	21449 [†]	20
Euro OTC	Prednisolone, micronized	1212021-02	21604 [†]	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
Fagron	Prednisolone, micronized	13H07-B02-285592	21660 [†]	20
Euro OTC	Prednisolone, micronized	1501047-01	21849 [†]	20
Caelo	Prednisolone, micronized	154000	22435 [†]	20
Caelo	Prednisolone, micronized	161343	22467 [†]	20
Euro OTC	Prednisolone, micronized	1702020	23180	40
Fagron	Prednisolone, micronized	16E09-B07-328220	23260	40
Caelo	Prednisolone, micronized	172777	23846	40
Caelo	Prednisolone, micronized	13343105	21451SI	60
Euro OTC	Prednisolone, micronized	1212021-02	21604SI [†]	15
Fagron	Prednisolone, micronized	13H07-B02-285592	21660SI [†]	20
Euro OTC	Prednisolone, micronized	1501047-01	21849SI [†]	10
Caelo	Prednisolone, micronized	154000	22435SI [†]	20
Caelo	Prednisolone, micronized	161343	22467SI [†]	16
Euro OTC	Prednisolone, micronized	1702020	23180SI	21
Fagron	Prednisolone, micronized	16E09-B07-328220	23260SI	20
Caelo	Prednisolone, micronized	172777	23846SI	38

- 126 392 spectra from a total of 2779 batches from further 781 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.

- 926 spectra from 314 *Apo-Ident* customers from 237 batches from the substance/substance group *Prednisolone, micronized*.

Supplier	Substance	Batch	Spectra
Fagron	Prednisolone, micronized	11D13-N05	1
EuRho	Prednisolone, micronized	1012012-02	2
Caelo	Prednisolone, micronized	10196622	2
Caelo	Prednisolone, micronized	10196626	6
EuRho	Prednisolone, micronized	1012012-01	1
Caelo	Prednisolone, micronized	10196627	7
Gehe	Prednisolone, micronized	12C22-N05	1
Fagron	Prednisolone, micronized	11J26-N04	2
Caelo	Prednisolone, micronized	11/26-N04	1
Fagron	Prednisolone, micronized	12C22-N05	7
europa	Prednisolone, micronized	1002001240	1
Euro OTC	Prednisolone, micronized	1108055-02	2
Caelo	Prednisolone, micronized	10196625	1
Caelo	Prednisolone, micronized	12171301	6
Phoenix	Prednisolone, micronized	11j26-N04	2
Noweda	Prednisolone, micronized	10196626	2
Fagron	Prednisolone, micronized	12D30-N04	9
Caelo	Prednisolone, micronized	12185702	2
Caelo	Prednisolone, micronized	12171306	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
Fagron	Prednisolone, micronized	FP01409P	1
Fagron	Prednisolone, micronized	12D30-N04	1
Caelo	Prednisolone, micronized	12171303	2
Caelo	Prednisolone, micronized	12171302	1
Sanacorp	Prednisolone, micronized	1108055-03	1
Caelo	Prednisolone, micronized	12324202	9
Euro OTC	Prednisolone, micronized	1108055-03	10
EuRho	Prednisolone, micronized	1108055-03	2
Fagron	Prednisolone, micronized	11G22-N08	1
Euro OTC	Prednisolone, micronized	1012012-02	2
Caelo	Prednisolone, micronized	20021303	1
Europharm/Otto	Prednisolone, micronized	1108055-03	1
Caelo	Prednisolone, micronized	12324204	4
Europharm/Otto	Prednisolone, micronized	1108055-04	5
Caelo	Prednisolone, micronized	12324205	12
Euro OTC	Prednisolone, micronized	1108055-04	13
Caelo	Prednisolone, micronized	10196611	2
Euro OTC	Prednisolone, micronized	110805504	3
Gehe	Prednisolone, micronized	13A07-N14	2
Fagron	Prednisolone, micronized	12K14-N03	8
Fagron	Prednisolone, micronized	13A07-N14	6
Euro OTC	Prednisolone, micronized	1108055-01	1
Euro OTC	Prednisolone, micronized	NEPL110103	1
Caelo	Prednisolone, micronized	1234205	1
Fagron	Prednisolone, micronized	12c22-N05	1
Caelo	Prednisolone, micronized	12324207	4
EuRho/Jenne	Prednisolone, micronized	1108055-04	2
Caelo	Prednisolone, micronized	2413Q02105	1
A.H. 05.03.13 ek: 14,08EUR	Prednisolone, micronized	12D30-N04	1
Gehe	Prednisolone, micronized	12324216	2
Apotheke Mildenaue	Prednisolone, micronized	1108055-04	2
Caelo	Prednisolone, micronized	12324213	7
Caesar & Loretz GmbH	Prednisolone, micronized	12324205	1
Caelo	Prednisolone, micronized	12324216	8
Phönix	Prednisolone, micronized	13E15-N06	2
Phönix	Prednisolone, micronized	13A07N14	1
Fagron	Prednisolone, micronized	12324216	1
Caelo	Prednisolone, micronized	13A07-N14	1
Phönix Gotha	Prednisolone, micronized	12324213	1
Caelo	Prednisolone, micronized	12324217	5
Euro OTC	Prednisolone, micronized	118055-04	1
Fagron	Prednisolone, micronized	13E15-N06	14
Caelo	Prednisolone, micronized	13E15-N06	4
euroct/Gehe	Prednisolone, micronized	1212021-01	2
Phönix Gotha	Prednisolone, micronized	12324217	1
Phönix	Prednisolone, micronized	12324216	1
Sanacorp	Prednisolone, micronized	13E15-N06	1
Euro OTC	Prednisolone, micronized	1212021-01	25
Fagron	Prednisolone, micronized	4313E-02105	1
Caelo	Prednisolone, micronized	10196604	1
Fagron	Prednisolone, micronized	13E15-N06	1
Caelo	Prednisolone, micronized	4513U2105	1
Caelo	Prednisolone, micronized	1511011	1
Caelo	Prednisolone, micronized	12324203	3
Fagron	Prednisolone, micronized	K04C20121006	1
Fargo	Prednisolone, micronized	12D30-N04	1
Caelo	Prednisolone, micronized	12324219	7
Gehe	Prednisolone, micronized	13E15-No6	1
Sonnenberg-Apotheke	Prednisolone, micronized	12324219	1
Caelo	Prednisolone, micronized	12324221	2

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Supplier	Substance	Batch	Spectra
Fagron	Prednisolone, micronized	13DE15-N06	1
Caelo	Prednisolone, micronized	1232417	1
Caelo	Prednisolone, micronized	411092-1-P	1
Sanacorp	Prednisolone, micronized	12324221	1
Fagron	Prednisolone, micronized	13H07-B02-285593	3
Tianyao Pharma/Phönix	Prednisolone, micronized	NEPL110103	1
Phönix Gotha	Prednisolone, micronized	1232417	1
Caesar & Loretz GmbH	Prednisolone, micronized	12324219	1
Euro OTC	Prednisolone, micronized	1314Q2105	1
Gehe	Prednisolone, micronized	1212021-01	4
Caelo	Prednisolone, micronized	12324226	6
Euro OTC	Prednisolone, micronized	30042014B	1
Caelo	Prednisolone, micronized		2
Caelo	Prednisolone, micronized	12324220	1
Fagron	Prednisolone, micronized	13H07-B020	1
Caelo	Prednisolone, micronized	1212021-01	1
Fagron	Prednisolone, micronized	13H07-B02-285590	2
Caelo	Prednisolone, micronized	4712I-02105	1
Fagron	Prednisolone, micronized	13E13-N06	1
Euro OTC	Prednisolone, micronized	121202102	2
Euro OTC	Prednisolone, micronized	121021-01	1
Fagron	Prednisolone, micronized	K04C20121006	1
Euro OTC	Prednisolone, micronized	121202101	1
Fagron	Prednisolone, micronized	13A07N14	1
Caelo	Prednisolone, micronized	13343106	7
Caelo	Prednisolone, micronized	13343105	3
Fagron	Prednisolone, micronized	13J28-B06	2
Fagron	Prednisolone, micronized	13H07-B02-285593	1
Fagron	Prednisolone, micronized	13H07-B02-285592	3
Euro OTC	Prednisolone, micronized	1212021-02	24
Fagron	Prednisolone, micronized	13J28-B06-289670	3
Fagron	Prednisolone, micronized	613Q-02105	1
Caelo	Prednisolone, micronized	13343104	10
Phönix Gotha	Prednisolone, micronized	13343105	1
Caelo	Prednisolone, micronized	133414	1
Gehe	Prednisolone, micronized	13343107	1
Fagron	Prednisolone, micronized	13H7-B02-285590	1
Fagron	Prednisolone, micronized	13343106	1
anzag	Prednisolone, micronized	14B18-B05-294966	1
Caelo	Prednisolone, micronized	13343111	4
Tianyao Pharma/Phönix	Prednisolone, micronized	1212021-01	1
Fagron	Prednisolone, micronized	K04C20131102	1
Euro OTC	Prednisolone, micronized	13343104	1
Fagron	Prednisolone, micronized	13H07-B02	2
Caelo	Prednisolone, micronized	13343101	1
Caelo	Prednisolone, micronized	13343113	1
Caelo	Prednisolone, micronized	121202102	1
Phönix Gotha	Prednisolone, micronized	13343112	2
Berkel AHK	Prednisolone, micronized	13343115	1
Caelo	Prednisolone, micronized	13343114	4
Phönix	Prednisolone, micronized	14B18-B05-294966	1
Fagron	Prednisolone, micronized	130F-N04	1
Caelo	Prednisolone, micronized	13343115	9
Fagron	Prednisolone, micronized	14B18-B05-294966	10
Gehe	Prednisolone, micronized	14A30-B02-294968	1
Fagron	Prednisolone, micronized	14B18-B05	1
Fagron	Prednisolone, micronized	14A30-B02-294968	4
Fagron	Prednisolone, micronized	14B18-Bo5-294966	1
Fagron	Prednisolone, micronized	K04C20130203M	1
Caelo	Prednisolone, micronized	k04c20121219	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Prednisolone, micronized	13j28-b06-289670	1
Caelo	Prednisolone, micronized	13343112	1
Caelo	Prednisolone, micronized	13343107	1
Caesar&Loretz GmbH/Anzag	Prednisolone, micronized	13343112	1
Fagron	Prednisolone, micronized	1410-B03	1
Caelo	Prednisolone, micronized	13343116	4
Fagron	Prednisolone, micronized	1212021-02	2
Caelo	Prednisolone, micronized	14B18-B05-294966	2
Fagron	Prednisolone, micronized	14B18-B05-294969	2
Caelo	Prednisolone, micronized	10196606	1
Fagron	Prednisolone, micronized	14/10-B03-302265	3
Fagron	Prednisolone, micronized	14B18-B05294966	1
Caelo	Prednisolone, micronized	14G30-B14-302262	1
Phönix Gotha	Prednisolone, micronized	13343111	1
Fagron	Prednisolone, micronized	14110-B03302265	1
Fagron	Prednisolone, micronized	14/10B03302265	1
Sanacorp	Prednisolone, micronized	14/10-B03-302269	1
Fagron	Prednisolone, micronized	14G30-B14-302262	4
Gehe	Prednisolone, micronized	1212021-02	1
Fagron	Prednisolone, micronized	14L10-B03-302269	1
Noweda	Prednisolone, micronized	1212021-02	1
Caelo	Prednisolone, micronized	15055101	5
Gehe-Fragon	Prednisolone, micronized	14B18B05294966	1
Fischar/Gehe	Prednisolone, micronized	14A30-B02-294968	1
Fagron	Prednisolone, micronized	14I10-B03-302265	2
Caelo	Prednisolone, micronized	15055102	5
Fagron	Prednisolone, micronized	K04C20140502	1
sanacorp	Prednisolone, micronized	14/10-B03-302266	1
Euro OTC	Prednisolone, micronized	1501047-01	18
Fagron	Prednisolone, micronized	14/10-B03-302266	2
Caelo	Prednisolone, micronized	15206103	8
Fagron	Prednisolone, micronized	14I10-B03	1
Fagron	Prednisolone, micronized	15D14-B01-308425	3
Gehe	Prednisolone, micronized	1501047-01	2
Caelo	Prednisolone, micronized	1410B03302265	1
Caelo	Prednisolone, micronized	1234556	1
Fagron	Prednisolone, micronized	15D14-B01	1
Caelo	Prednisolone, micronized	15206102	18
Caelo/Noweda	Prednisolone, micronized	1526108	1
Caelo	Prednisolone, micronized	15206108	12
Fagron	Prednisolone, micronized		1
Fagron	Prednisolone, micronized	14I10-B03-302266	1
Euro OTC	Prednisolone, micronized	1212021-03	30
Fagron	Prednisolone, micronized	15K03-B04-314226	12
Noweda	Prednisolone, micronized	1108055-05	1
Caelo	Prednisolone, micronized	15206101	7
Euro OTC	Prednisolone, micronized	12021-03	1
Caelo	Prednisolone, micronized	15206105	7
Fagron	Prednisolone, micronized	15K03-B04-314358	6
Caesar & Loretz GmbH	Prednisolone, micronized	15206101	2
Caelo	Prednisolone, micronized	1212021-03	4
Fagron	Prednisolone, micronized	14/10-B03-302269	1
Euro OTC	Prednisolone, micronized	1212021	1
Caelo	Prednisolone, micronized	9193501	1
Fagron	Prednisolone, micronized	1410-B03-302269	2
Euro OTC	Prednisolone, micronized	150104701	2
Fagron	Prednisolone, micronized	15K03-B04-314226	1
Euro OTC	Prednisolone, micronized	121221-03	1
Noweda	Prednisolone, micronized	15206101	1
Fagron	Prednisolone, micronized	16A20-B03-316420	5

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Supplier	Substance	Batch	Spectra
Caelo	Prednisolone, micronized	15206106	1
Fagron	Prednisolone, micronized	15k03-b04-314226	1
Caelo	Prednisolone, micronized	152006105	1
Caelo	Prednisolone, micronized	150104701	2
Fagron/Phoenix	Prednisolone, micronized	15K03-B04-314226	1
Caelo	Prednisolone, micronized	15400003	19
Caelo	Prednisolone, micronized	15400002	17
Caelo	Prednisolone, micronized	14A30-B02-294968	1
Fagron	Prednisolone, micronized	15B18-B05-294969	1
Euro OTC	Prednisolone, micronized	150104747-01	1
AHD	Prednisolone, micronized	121202103	1
Caelo	Prednisolone, micronized	1501047-01	3
Phoenix	Prednisolone, micronized	15400003	1
Fagron	Prednisolone, micronized	16A20-B03-319015	5
Caelo	Prednisolone, micronized	15K03-B04-314358	1
Euro OTC	Prednisolone, micronized	1501047-02	12
Fagron	Prednisolone, micronized	16A20-B03	4
Bombastus	Prednisolone, micronized	1501047-02	1
Fagron	Prednisolone, micronized	15K03B04314226	1
Sanacorp WE:01.08.2016 ...	Prednisolone, micronized	1501047-01	1
Euro/ Sanacorp	Prednisolone, micronized	121202103	1
Euro OTC	Prednisolone, micronized	501047-01	1
Caelo	Prednisolone, micronized	1501047-02	2
Caolo- Noweda	Prednisolone, micronized	15206103	1
Fagron	Prednisolone, micronized	14I10-B03-302269	1
Fagron	Prednisolone, micronized	16A20-B03-316421	1
Euro OTC	Prednisolone, micronized	1501047	1
Fagron	Prednisolone, micronized	15K03-B04-314357	2
Fagron	Prednisolone, micronized	150528P	1
Caelo	Prednisolone, micronized	15400004	14
Caelo	Prednisolone, micronized	1540003	1
Fagron	Prednisolone, micronized	16C15-B01-321979	8
Euro OTC	Prednisolone, micronized	15010477-01	1
Henan Lihua/Gehe	Prednisolone, micronized	1501047-01	1
Fagron	Prednisolone, micronized	16c15-B01-320761	1
Euro OTC	Prednisolone, micronized	1607011-01	18
Caelo	Prednisolone, micronized	16C15-B01-320761	1
Caelo	Prednisolone, micronized	16C15-B01-321979	2
Caelo	Prednisolone, micronized	16C15-B01320761	1
Fagron	Prednisolone, micronized	16C15-B01-320761	1
Caelo	Prednisolone, micronized	16A20-B03-316421	1
Fagron	Prednisolone, micronized	16C15-B01-324942	4
Caelo	Prednisolone, micronized	15400001	2
Gehe	Prednisolone, micronized	16C15-B01	1
Fagron	Prednisolone, micronized	16C15B01320761	1
Ichthyol / Phoenix	Prednisolone, micronized	16C15-B01-320761	1
Caelo	Prednisolone, micronized	16134302	10
Fagron	Prednisolone, micronized	16C15-B01-319992	1
Fagron	Prednisolone, micronized	16C15B01321979	1
Caelo	Prednisolone, micronized	NEPL160202	1
Fagron	Prednisolone, micronized	NEPL151202	1
Caelo	Prednisolone, micronized	16134301	4
Fagron	Prednisolone, micronized	16C15-B01	1
Fagron	Prednisolone, micronized	16C15-B02-324943	4
Fagron	Prednisolone, micronized	16C15-B01-321979	1
Fagron	Prednisolone, micronized	16E09-B07-328150	6
Gehe	Prednisolone, micronized	16C-15-B02	1
Caelo	Prednisolone, micronized	16134305	8
Fagron	Prednisolone, micronized	1717M-02105	1
Fagron	Prednisolone, micronized	16C15-B02-324945	1

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Supplier	Substance	Batch	Spectra
Fagron	Prednisolone, micronized	16E09/B07/328220	1
Gehe	Prednisolone, micronized	16134302	1
Gehe	Prednisolone, micronized	16E09-B07	1
AHD	Prednisolone, micronized	160711-01	1
Euro OTC	Prednisolone, micronized	16134308	3
Caelo	Prednisolone, micronized	16134306	4
Caelo	Prednisolone, micronized	15400010	1
Caelo	Prednisolone, micronized	16E09-B07-328150	2
Fagron	Prednisolone, micronized	16E09-B07328220	1
Fagron	Prednisolone, micronized	1607011-01	2
Noweda	Prednisolone, micronized	1607011-01	1
Fagron	Prednisolone, micronized	16E09-B07-328220	2
Fagron	Prednisolone, micronized	16H04-B03-332929	8
Gehe/Fragon	Prednisolone, micronized	16E09B07328150	1
Caelo	Prednisolone, micronized	16134308	5
Caelo	Prednisolone, micronized	16134310	9
Fagron	Prednisolone, micronized	16E09-B07-329686	1
Caelo	Prednisolone, micronized	16134303	1
Euro OTC	Prednisolone, micronized	1702020-01	13
Fagron	Prednisolone, micronized	16E09-B075411	1
Bomastus / Alliance Hea...	Prednisolone, micronized	16134305	1
Fagron	Prednisolone, micronized	16C15-B02	1
Caelo	Prednisolone, micronized	18138113	1
Caelo	Prednisolone, micronized	1613414	1
Fargon	Prednisolone, micronized	16134308	1
Fagron	Prednisolone, micronized	16H04-B03-332930	3
Caelo	Prednisolone, micronized	16134314	6
Caelo	Prednisolone, micronized	16134316	11
Sanacorp	Prednisolone, micronized	16H04-B03332930	1
Fagron	Prednisolone, micronized	17F07-B05-341575	2
AHD	Prednisolone, micronized	1702020-01	1
Caelo	Prednisolone, micronized	17020-01	1
Fagron	Prednisolone, micronized	17D14-B01	1
EuRho/Noweda	Prednisolone, micronized	1702020-01	1
Euro OTC	Prednisolone, micronized	1702020-02	6
Bombastus	Prednisolone, micronized	17F07-B05-341574	2
GEHE	Prednisolone, micronized	1702020-02	1
Fagron	Prednisolone, micronized	17F07-B05-341574	2
Fagron	Prednisolone, micronized	17F07-B05	1
Fagron	Prednisolone, micronized	14/10-B03	1
Fagron	Prednisolone, micronized	NEPL170209	1
Fagron	Prednisolone, micronized	NEPL170210	1
Fagron	Prednisolone, micronized	17G28-B03-345539	1
Fagron	Prednisolone, micronized	17D14-B01-338573	1
Euro OTC	Prednisolone, micronized	1501047-03	2
Caelo	Prednisolone, micronized	16134315	2
Fagron	Prednisolone, micronized	17G28-B03-345538	2
Fagron	Prednisolone, micronized	17D14-Bo1-338573	1
Caelo	Prednisolone, micronized	1702020-01	1
Sanacorp	Prednisolone, micronized	18AB02	1
Fargon/AHD	Prednisolone, micronized	18A29-B02-348044	1
Fagron	Prednisolone, micronized	18A29-B02-348540	1
Fagron	Prednisolone, micronized	18C19-B07-351226	1
Caelo	Prednisolone, micronized	17F07-B05-341578	1
Fagron	Prednisolone, micronized	17F07-B05-341578	1
Fagron	Prednisolone, micronized	18C19-B07-353242	1
Caelo	Prednisolone, micronized	17277704	3
Euro OTC	Prednisolone, micronized	1702020-03	1
Caelo	Prednisolone, micronized	17277703	3
Caelo	Prednisolone, micronized	17277702	1

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Supplier	Substance	Batch	Spectra
Fagron	Prednisolone, micronized	18H07-B04-354523	1
Caelo	Prednisolone, micronized	NEPL180603	1
Fagron	Prednisolone, micronized	18H07-B04	1

- 78 003 spectra from 565 *Apo-Ident* customers from a total of 25 902 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Prednisolone, micronized* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisolone, micronized* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	798	0	73 698
Type B	0	500	0	126 392
Type C	0	924	2	78 003

The substance/substance group *Prednisolone, micronized* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 99.2481 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.8000 %)
Type C	100.0000 % (> 99.8817 %)	99.7840 % (> 99.4600 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
20773	21303	5.74	40.64

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21604	21604	0.00	38.00
22651	21303	5.56	39.95
21660	21449	1.59	34.18
21449	21449	0.00	33.79
21849	21849	0.00	27.25
22709	22709	0.00	31.78
22783	22435	2.69	37.74
22803	22435	4.29	36.33
21303	21303	0.00	34.47
22435	22435	0.00	38.04
22467	22467	0.00	26.71

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Prednisone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20002-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Prednisone; Prednisonum

Special notes

When selecting the *Prednisone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Prednisone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisone	12232716	21408	40	20120829
Euro OTC	Prednisone	1401042-02	21616	40	1605276
Euro OTC	Prednisone	1604051	22557	40	20160523*
Fagron	Prednisone	16J19-B02-328642	23227	40	20161221
Caelo	Prednisone	12232716	21408SI	40	20120829
Euro OTC	Prednisone	1604051	22557SI	40	20160523*

Validation samples

A total of 280 317 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 *Prednisone*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1619 batches from further 372 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 [†].

- 449 spectra of 13 reference samples from the substance/substance group *Prednisone*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednisone	12232716	21408 [†]	20
Caelo	Prednisone	12232716	21409	60
Fagron	Prednisone	13C14-B40-289148	21573	60
Euro OTC	Prednisone	1401042-02	21616 [†]	20
Euro OTC	Prednisone	1702008	23179	40
Caelo	Prednisone	171665	23341	20
Caelo	Prednisone	17166504	23578	30
Caelo	Prednisone	12232716	21408SI [†]	20
Caelo	Prednisone	12232716	21409SI	60
Euro OTC	Prednisone	1702008	23179SI	29
Fagron	Prednisone	16J19-B02-328642	23227SI	30
Caelo	Prednisone	171665	23341SI	30
Caelo	Prednisone	17166504	23578SI	30

- 126 443 spectra from a total of 2782 batches from further 781 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.

- 49 spectra from 30 *Apo-Ident* customers from 34 batches from the substance/substance group *Prednisone*.

Supplier	Substance	Batch	Spectra
Caelo	Prednisone	12177604	1
Caelo	Prednisone	204312107	1
Phönix	Prednisone	11D08-N05	1
Gehe	Prednisone	12L14-M03	1
Caelo	Prednisone	10037817	1
Caelo	Prednisone	10037826	1
Fagron	Prednisone	13C13-N08	1
Caelo	Prednisone	12232705	3
Fagron	Prednisone	21021401	1
Gehe	Prednisone	13C13-N08	1
Fagron	Prednisone	12E02-N01	1
Gehe	Prednisone	12232714	1
Caelo	Prednisone	2114Q2107	1
Fagron	Prednisone	12E02-N10	1
Caelo	Prednisone	12232714	1
Caelo	Prednisone	5087	1
Caelo	Prednisone	12232713	1
sanacorp	Prednisone	13262302	1
Euro OTC	Prednisone	1401042-02	1
Caelo	Prednisone	15218602	4
Caelo	Prednisone	13262304	1
Caelo	Prednisone	15218607	1
Caelo	Prednisone	15218606	3
Fagron	Prednisone	15218608	1
Euro OTC	Prednisone	1501043-03	4
Caelo	Prednisone	16277201	1
Caelo	Prednisone	16277206	1
Euro OTC	Prednisone	1501043-02	1
Euro OTC	Prednisone	1604501-01	1
Euro OTC	Prednisone	150043-03	1
Sanacorp	Prednisone	16277206	1
Caelo	Prednisone	17166502	1
Fagron	Prednisone	16H04-B04-334368	1
Caelo	Prednisone	17166507	3
Caelo	Prednisone	17166504	1
Euro OTC	Prednisone	1604051-01	1
Euro OTC	Prednisone	1702008-01	1

- 78 880 spectra from 565 *Apo-Ident* customers from a total of 26 103 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Prednisone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	449	0	126 443
Type C	0	48	1	78 880

The substance/substance group *Prednisone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.6637 %)
Type C	100.0000 % (> 99.8817 %)	97.9592 % (> 91.8367 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22557	22557	0.00	23.26
21616	21616	0.00	19.87
23227	22557	4.24	26.39
21408	22557	9.84	25.78

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Pregnenolone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20721-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Pregnenolone; Pregnenolonum

Special notes

When selecting the *Pregnenolone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Pregnenolone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Pregnenolone	1204040-01	20721	40	1404311
Euro OTC	Pregnenolone	1312007-01	21679	40	8985
Fagron	Pregnenolone	15B11-B07-310278	22355	30	9338
Euro OTC	Pregnenolone	1602001	22375	30	20160208*
Euro OTC	Pregnenolone	1612019	22979	40	20170131*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 5 reference samples from the substance/substance group *Pregnenolone*. These samples are listed above in the [calibration samples](#) section.
- 74 316 spectra from a total of 1618 batches from further 372 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 5 reference samples from the substance/substance group *Pregnenolone*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Pregnenolone	1312007-01	21679 [†]	20
Fagron	Pregnenolone	15B11-B07-310278	22355 [†]	15
Euro OTC	Pregnenolone	1602001	22375 [†]	15
Euro OTC	Pregnenolone	1606028	22706	40
Euro OTC	Pregnenolone	1709017	23696	40

- 126 762 spectra from a total of 2784 batches from further 781 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*.

- 21 spectra from 10 *Apo-Ident* customers from 19 batches from the substance/substance group *Pregnenolone*.

Supplier	Substance	Batch	Spectra
Audor Pharma	Pregnenolone	AP1109007-01P	1
Audor Pharma	Pregnenolone	AP10L10-M01P	1
KS Pharma	Pregnenolone	ZH-111119	1
Euro OTC	Pregnenolone	1312007-01	1
Haihang Industry	Pregnenolone	20140329	1
Koisser	Pregnenolone	ZH-130802	1
Koisser Pharma	Pregnenolone	ZH-131001	1
Euro OTC	Pregnenolone	1402025-01	1
Fagron	Pregnenolone	14B18-B04-291917	1
NWM Shandong Northwest ...	Pregnenolone	PRN151219	1
Audor Pharma	Pregnenolone	APC07-150801(M)P	2
NWM CHina	Pregnenolone	PR150329	1
Euro OTC	Pregnenolone	1602001-01	1
Euro OTC	Pregnenolone	1612019-01	1
Fagron	Pregnenolone	16L29-B02331611	1
Audor Pharma	Pregnenolone	APC07-160801(M)P	1
gehe	Pregnenolone	Apc07160801	1
Audor Pharma	Pregnenolone	APC07-180201(M)P	2
Audor Pharma	Pregnenolone	APC07-180201	1

- 78 908 spectra from 565 *Apo-Ident* customers from a total of 26 118 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Pregnenolone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pregnenolone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	180	0	74 316
Type B	0	130	0	126 762
Type C	0	21	0	78 908

The substance/substance group *Pregnenolone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 71.4286 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22979	22979	0.00	22.08
20721	20721	0.00	24.25
22355	22355	0.00	23.12
21679	21679	0.00	21.75
22375	22375	0.00	22.21

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Prilocaine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21048-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Prilocaine hydrochloride; Prilocaini hydrochloridum

Special notes

When selecting the *Prilocaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Prilocaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Prilocaine hydro...	13I02-N03	21048	40	1403257
Fagron	Prilocaine hydro...	14H13-B03-297591	21800	40	AR-15-FG-016323-01
Caelo	Prilocaine hydro...	15230305	21926	40	20150723

Validation samples

A total of 280 317 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 *Prilocaine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 [†].

- 273 spectra of 7 reference samples from the substance/substance group *Prilocaine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Prilocaine hydrochloride	13I02-N03	21050	40
Fagron	Prilocaine hydrochloride	14H13-B03-297591	21800 [†]	20
Caelo	Prilocaine hydrochloride	15230305	21926 [†]	20
Caelo	Prilocaine hydrochloride	15390101	23250	40
Fagron	Prilocaine hydrochloride	14H13-B03-297591	21800SI	60
Caelo	Prilocaine hydrochloride	15230305	21926SI	60
Caelo	Prilocaine hydrochloride	15390101	23250SI	33

- 126 619 spectra from a total of 2785 batches from further 781 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 *Prilocaine hydrochloride*.

[†]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	Prilocaine hydrochloride	14A03-B34-290281	1
GEHE 02.05.2013	Prilocaine hydrochloride		1
Fagron	Prilocaine hydrochloride	14H13-B03-297591	1
Fagron	Prilocaine hydrochloride	13I032-N03	1
Fagron	Prilocaine hydrochloride	17H02-B05	1
Fagron	Prilocaine hydrochloride	15L21-B02325756	1

- 78 923 spectra from 565 *Apo-Ident* customers from a total of 26 131 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Prilocaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prilocaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	261	12	126 619
Type C	0	6	0	78 923

The substance/substance group *Prilocaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	95.6044 % (> 94.5055 %)
Type C	100.0000 % (> 99.8819 %)	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
21048	21048	0.00	45.55
21800	21800	0.00	54.82
21926	21800	6.36	54.94

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Procaine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20042-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Procaine hydrochloride; Procaini hydrochloridum

Special notes

When selecting the *Procaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Procaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Procaine hydroch...	13109906	21785	40	AR-15-FG-008935-01
Caelo	Procaine hydroch...	15006906	22247	40	20150209
Fagron	Procaine hydroch...	13F12-B40-301798	22260	40	20141210
Euro OTC	Procaine hydroch...	1601014	22306	40	20160203*

Validation samples

A total of 280317 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 *Procaine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 8 reference samples from the substance/substance group *Procaine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Procaine hydrochloride	13109906	21785 [†]	20
Caelo	Procaine hydrochloride	15006906	22247 [†]	20
Fagron	Procaine hydrochloride	13F12-B40-301798	22260 [†]	20
Euro OTC	Procaine hydrochloride	1601014	22306 [†]	20
Caelo	Procaine hydrochloride	161378	22624	40
Fagron	Procaine hydrochloride	15J27-B10-322937	23379	40
Caelo	Procaine hydrochloride	171675	23634	40
Caelo	Procaine hydrochloride	182764	24393	40

- 126652 spectra from a total of 2781 batches from further 781 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.

- 92 spectra from 63 *Apo-Ident* customers from 56 batches from the substance/substance group *Procaine hydrochloride*.

Supplier	Substance	Batch	Spectra
Caelo	Procaine hydrochloride	10159723	1
Euro OTC	Procaine hydrochloride	1104012-01	1
Caelo	Procaine hydrochloride	10159729	1
Anzag	Procaine hydrochloride	60998058	1
Euro OTC	Procaine hydrochloride	200644	1
Caelo	Procaine hydrochloride	11370203	1
Caelo	Procaine hydrochloride	11370204	1
Caelo	Procaine hydrochloride	11370206	1
Caelo	Procaine hydrochloride	12177801	5
Caelo	Procaine hydrochloride	10159721	1
Caelo	Procaine hydrochloride	11370215	1
Euro OTC	Procaine hydrochloride	1104012-03	3
Euro OTC	Procaine hydrochloride	1003001-01	1
Herstellung	Procaine hydrochloride	12177801	1
Caelo	Procaine hydrochloride	11370216	2
Caelo	Procaine hydrochloride	11370219	1
Caelo	Procaine hydrochloride	131099903	1
Koisser	Procaine hydrochloride	11370218	1
Fagron	Procaine hydrochloride	1651212	1
Fagron	Procaine hydrochloride	12I10-N07	1
Fagron	Procaine hydrochloride	10H11-N25	1
Caelo	Procaine hydrochloride	60998127	2
Caelo	Procaine hydrochloride	13109908	2
Euro OTC	Procaine hydrochloride	1104012-04	3
Phönix 08.01.2014	Procaine hydrochloride	1104012-03	1
China Medica	Procaine hydrochloride	13109911	1
Phönix Gotha	Procaine hydrochloride	190311	1
siehe WE-Prüfprotokoll	Procaine hydrochloride	39/12	1
Caelo	Procaine hydrochloride	13109915	1
Fagron	Procaine hydrochloride	13I09-N08	1
Euro OTC	Procaine hydrochloride	1104012-05	4
Caelo	Procaine hydrochloride	13109906	1
Caelo	Procaine hydrochloride	13/09-N08	1
Alliance Health 09.09.2...	Procaine hydrochloride	1104012-05	1
Gatt-Koller / Phoenix	Procaine hydrochloride	4428/10122714	2
Euro OTC	Procaine hydrochloride	5127	1
Caelo	Procaine hydrochloride	13109905	1
Fagron	Procaine hydrochloride	13/30-N06	1
Caelo	Procaine hydrochloride	7011506	1
Caelo	Procaine hydrochloride	13109916	2
Caelo	Procaine hydrochloride	14164408	1
Euro OTC	Procaine hydrochloride	1405027-01	4
Caelo	Procaine hydrochloride	15006902	1
Caelo	Procaine hydrochloride	14164409	1
Euro OTC	Procaine hydrochloride	1405027-02	1
Noweda	Procaine hydrochloride	1309N08	1
Fagron	Procaine hydrochloride	13F12-B40	1
Caesar & Loretz GmbH	Procaine hydrochloride	14164413	1
Caelo	Procaine hydrochloride	15006906	3
Caelo	Procaine hydrochloride	13F12-B40-302510	1
Caelo	Procaine hydrochloride	14164413	1
Euro OTC	Procaine hydrochloride	1601014-01	7
Caelo	Procaine hydrochloride	15006913	1
Fagron	Procaine hydrochloride	15006906	1

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Supplier	Substance	Batch	Spectra
Caelo	Procaine hydrochloride	15006912	2
Caelo	Procaine hydrochloride	13130-N06	1
Caelo	Procaine hydrochloride	16173906	1
Caelo	Procaine hydrochloride	16137812	2
Caelo	Procaine hydrochloride	17167504	1
Euro OTC	Procaine hydrochloride	1601014-02	3
Caelo	Procaine hydrochloride	18041806	1

- 78 837 spectra from 565 *Apo-Ident* customers from a total of 26 081 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Procaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Procaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	235	5	126 652
Type C	0	91	1	78 837

The substance/substance group *Procaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	97.9167 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	98.9130 % (> 95.6522 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21785	21785	0.00	44.59
22247	21785	3.77	47.37
22260	21785	3.37	46.94
22306	22306	0.00	45.57

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Progesterone, micronized**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20024-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Progesterone, micronized; Progesteronum micronisatum

Special notes

When selecting the *Progesterone, micronized* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Progesterone, micronized*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Progesterone, mi...	1111053-01	20718	30	20120119
Euro OTC	Progesterone, mi...	1506033	21868	20	0000010482
Euro OTC	Progesterone, mi...	1506034	21870	40	0000010483
Euro OTC	Progesterone, mi...	1509008	21907	40	20150914*
Euro OTC	Progesterone, mi...	1511008	22226	40	20151119*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Progesterone, mi...	1601009	22301	30	20160128*
Euro OTC	Progesterone, mi...	1601001	22303	30	20160128*
Euro OTC	Progesterone, mi...	1603004	22525	40	20160406*
Fagron	Progesterone, mi...	16A20-B02-319103	22830	40	20160209
Caelo	Progesterone, mi...	15319601	22831	40	20151014
Euro OTC	Progesterone, mi...	1506033	21868SI	20	0000010482
Euro OTC	Progesterone, mi...	1601009	22301SI	30	20160128*
Fagron	Progesterone, mi...	16A20-B02-319103	22830SI	40	20160209

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 13 reference samples from the substance/substance group *Progesterone, micronized*. These samples are listed above in the [calibration samples](#) section.
- 74 056 spectra from a total of 1613 batches from further 372 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 [†].

- 2089 spectra of 62 reference samples from the substance/substance group *Progesterone, micronized*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Progesterone, micronized	1506033	21868 [†]	40
Euro OTC	Progesterone, micronized	1506034	21870 [†]	20
Euro OTC	Progesterone, micronized	1509008	21907 [†]	20
Euro OTC	Progesterone, micronized	1511008	22226 [†]	20
Euro OTC	Progesterone, micronized	1601009	22301 [†]	15
Euro OTC	Progesterone, micronized	1601001	22303 [†]	15
Euro OTC	Progesterone, micronized	1603012	22529	40
Euro OTC	Progesterone, micronized	1605013	22556	40
Euro OTC	Progesterone, micronized	1606033	22704	40
Euro OTC	Progesterone, micronized	1605032	22705	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
Euro OTC	Progesterone, micronized	1609016	22788	40
Euro OTC	Progesterone, micronized	1609001	22819	40
Euro OTC	Progesterone, micronized	1701038	23138	40
Euro OTC	Progesterone, micronized	1702026	23148	40
Caelo	Progesterone, micronized	17060903	23249	40
Caelo	Progesterone, micronized	170609	23329	40
Euro OTC	Progesterone, micronized	1707012	23536	40
Euro OTC	Progesterone, micronized	1705028	23541	40
Euro OTC	Progesterone, micronized	1709012	23732	40
Caelo	Progesterone, micronized	172778	23838	40
Caelo	Progesterone, micronized	170609	23844	40
Euro OTC	Progesterone, micronized	1801036	23947	40
Euro OTC	Progesterone, micronized	1802030	24067	40
Euro OTC	Progesterone, micronized	1806020	24138	40
Euro OTC	Progesterone, micronized	1809018	24328	40
Euro OTC	Progesterone, micronized	1809017	24334	40
Euro OTC	Progesterone, micronized	1603012-01	24335	40
Euro OTC	Progesterone, micronized	1811033	24345	40
Euro OTC	Progesterone, micronized	1901021	24447	40
Euro OTC	Progesterone, micronized	1901022	24455	40
Euro OTC	Progesterone, micronized	1506033	21868SI [†]	30
Euro OTC	Progesterone, micronized	1506034	21870SI	59
Euro OTC	Progesterone, micronized	1509008	21907SI	53
Euro OTC	Progesterone, micronized	1511008	22226SI	27
Euro OTC	Progesterone, micronized	1601009	22301SI [†]	15
Euro OTC	Progesterone, micronized	1601001	22303SI	44
Euro OTC	Progesterone, micronized	1603004	22525SI	31
Euro OTC	Progesterone, micronized	1603012	22529SI	29
Euro OTC	Progesterone, micronized	1605013	22556SI	30
Euro OTC	Progesterone, micronized	1606033	22704SI	30
Euro OTC	Progesterone, micronized	1605032	22705SI	38
Euro OTC	Progesterone, micronized	1609016	22788SI	30
Euro OTC	Progesterone, micronized	1609001	22819SI	30
Caelo	Progesterone, micronized	15319601	22831SI	40
Euro OTC	Progesterone, micronized	1701038	23138SI	20
Euro OTC	Progesterone, micronized	1702026	23148SI	20
Caelo	Progesterone, micronized	17060903	23249SI	20
Caelo	Progesterone, micronized	170609	23329SI	20
Euro OTC	Progesterone, micronized	1707012	23536SI	28
Euro OTC	Progesterone, micronized	1705028	23541SI	25
Euro OTC	Progesterone, micronized	1709012	23732SI	40
Caelo	Progesterone, micronized	172778	23838SI	30
Caelo	Progesterone, micronized	170609	23844SI	23
Euro OTC	Progesterone, micronized	1801036	23947SI	20
Euro OTC	Progesterone, micronized	1802030	24067SI	32
Euro OTC	Progesterone, micronized	1806020	24138SI	35
Euro OTC	Progesterone, micronized	1809018	24328SI	30
Euro OTC	Progesterone, micronized	1809017	24334SI	40
Euro OTC	Progesterone, micronized	1603012-01	24335SI	20
Euro OTC	Progesterone, micronized	1811033	24345SI	30
Euro OTC	Progesterone, micronized	1901021	24447SI	40
Euro OTC	Progesterone, micronized	1901022	24455SI	40

[†]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*.

- 124 803 spectra from a total of 2758 batches from further 781 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.

- 782 spectra from 192 *Apo-Ident* customers from 266 batches from the substance/substance group *Progesterone, micronized*.

Supplier	Substance	Batch	Spectra
Caelo	Progesterone, micronized	9195408	1
Euro OTC	Progesterone, micronized	1111053-01	6
Klenk	Progesterone, micronized	C01-120322	1
Caelo	Progesterone, micronized	11177221	2
Caelo	Progesterone, micronized	11177207	1
Fagron	Progesterone, micronized	1910213235	1
Caelo	Progesterone, micronized	9195429	1
Fagron	Progesterone, micronized	12D05-N06	3
Caelo	Progesterone, micronized	12195905	3
Euro OTC	Progesterone, micronized	1206024-01	1
Caelo	Progesterone, micronized	11177219	3
ANZAG	Progesterone, micronized	12195907	2
Fagron	Progesterone, micronized	12G05-N17	6
Caelo	Progesterone, micronized	12195907	4
Caelo	Progesterone, micronized	12195906	4
Fagron	Progesterone, micronized	12K05-N01	2
Caelo	Progesterone, micronized	12195913	3
Euro OTC	Progesterone, micronized	1211004-01	5
Fagron	Progesterone, micronized	12A19-N04	2
Caelo	Progesterone, micronized	12195920	8
Caelo	Progesterone, micronized	12195914	2
Fagron	Progesterone, micronized	13A02N01	1
Fagron	Progesterone, micronized	12K05-N07	1
Caelo	Progesterone, micronized	12195926	19
Euro OTC	Progesterone, micronized	co1-111218(M)	1
Caelo	Progesterone, micronized	C01-120613	1
A.H. 03.06.13 ek: 6,50EUR	Progesterone, micronized	1304014-01	1
Euro OTC	Progesterone, micronized	1304040-01	4
Fagron	Progesterone, micronized	1-111218	1
Sanacorp	Progesterone, micronized	12195914	1
Fagron	Progesterone, micronized	12k05-n07	1
Euro OTC	Progesterone, micronized	C01-130301M	1
Fragon	Progesterone, micronized	13A02-N02	1
Fagron	Progesterone, micronized	C01-120322	1
Caelo	Progesterone, micronized	12195928	7
Fagron	Progesterone, micronized	13A02-N01	3
Euro OTC	Progesterone, micronized	1304040-02	2
Caelo	Progesterone, micronized	130404002	2
Audor Pharma	Progesterone, micronized	C01-120708P	1
Euro OTC	Progesterone, micronized	130404001	1
Fagron	Progesterone, micronized	13G11-N02	4
Sanacorp	Progesterone, micronized	13A02-N01	1
Sanacorp	Progesterone, micronized	12195928	1
Fagron	Progesterone, micronized	13b08-n01	1
Caelo	Progesterone, micronized	12195912	3

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Supplier	Substance	Batch	Spectra
Alliance Healthcare	Progesterone, micronized	1206024-02	1
Audor Pharma	Progesterone, micronized	APC01-120708P	3
EuRho	Progesterone, micronized	1304040-02	1
Caelo	Progesterone, micronized	13155902	10
AHD	Progesterone, micronized	13I11-N11	1
Euro OTC	Progesterone, micronized	c01-130301	1
Euro OTC	Progesterone, micronized	c01-111218	1
Fagron	Progesterone, micronized	13/11-N11	1
Fagron	Progesterone, micronized	13I11-N11	2
Euro OTC	Progesterone, micronized	C01-130301(M)	2
Euro OTC	Progesterone, micronized	1308015-01	2
Fagron	Progesterone, micronized	C01-130301	1
Euro OTC	Progesterone, micronized		1
Sanacorp	Progesterone, micronized	13155902	1
China Medica	Progesterone, micronized	1308015-01	1
PHOENIX am 18.03.2014	Progesterone, micronized	13A02-N01	1
Audor Pharma	Progesterone, micronized	APC01-120613P	1
Fagron	Progesterone, micronized	13H01-N03	5
Fagron	Progesterone, micronized	13K-B30-288261	1
Phoenix 28.03.2014	Progesterone, micronized	13G11-N02	1
Fagron	Progesterone, micronized	1311-N11	1
Caelo	Progesterone, micronized	140100201	1
Vdl 28.04.14;Preis 39,95	Progesterone, micronized		1
Caelo	Progesterone, micronized	12195828	1
Changzhou Jiaerke Pharma	Progesterone, micronized	1308015-01	1
	Progesterone, micronized	1401002-01	2
Fagron	Progesterone, micronized	13K28-B30-288262	1
Fagron	Progesterone, micronized	13K28-B30-288261	1
Euro OTC	Progesterone, micronized	1403019-01	2
Caelo	Progesterone, micronized	13155921	2
Fagron	Progesterone, micronized	5013I-03235	1
Euro OTC	Progesterone, micronized	1401002-01	1
Euro/ Sanacorp	Progesterone, micronized	C01-131116(M)	1
Euro OTC	Progesterone, micronized	1406022-01	1
Anzag	Progesterone, micronized	13K28-B01-293478	1
Fagron	Progesterone, micronized	14022-B04-293476	1
Euro OTC	Progesterone, micronized	1406022-02	2
Fagron	Progesterone, micronized	14C10B0129347	1
Caelo	Progesterone, micronized	13155927	2
Euro OTC	Progesterone, micronized	7406022-01	1
Caelo	Progesterone, micronized	13155920	1
Phönix	Progesterone, micronized	13155920	1
Caelo	Progesterone, micronized	13155928	3
Euro OTC	Progesterone, micronized	140602202	1
Euro OTC	Progesterone, micronized	5102	1
Euro OTC	Progesterone, micronized	5104	1
Euro OTC	Progesterone, micronized	140910-01	1
Fagron	Progesterone, micronized	14D22-Bo4	1
Fagron	Progesterone, micronized	14c10-B01-293478	1
Fagron	Progesterone, micronized	14c10-b01-293478	1
Fagron	Progesterone, micronized	14D22-B04	2
Fagron	Progesterone, micronized	13h01-n03	1
VDL;07.11.14;39,95 euro	Progesterone, micronized	13155921	1
Fagron	Progesterone, micronized	14C10-B01-293478	2
Phoenix 09.12.14	Progesterone, micronized	13H01-N03	1
Euro OTC	Progesterone, micronized	1409029-1	1
Caelo	Progesterone, micronized	13155929	1
Euro OTC	Progesterone, micronized	1409029-01	3
Euro OTC	Progesterone, micronized	1406910-01	1
Euro OTC	Progesterone, micronized	1411043-01	4

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Supplier	Substance	Batch	Spectra
Fagron	Progesterone, micronized	14D22-B04-293477	1
Euro OTC	Progesterone, micronized	1409019-01	1
Fagron	Progesterone, micronized	14C10-B01	1
Caesar/Noweda	Progesterone, micronized	12195912	1
Caelo	Progesterone, micronized	13HI01-N03	1
Fagron	Progesterone, micronized	14K11-B04-300920	6
Euro OTC	Progesterone, micronized	1502030-01	2
Fagron	Progesterone, micronized	14H13-B05-300216	7
	Progesterone, micronized	14253906	1
Fagron	Progesterone, micronized	HTT140302	1
Caelo	Progesterone, micronized	HTT140302	1
Caelo	Progesterone, micronized	14253911	2
Anzag	Progesterone, micronized	2515A-03235	1
Fagron	Progesterone, micronized	14D22-B293479	1
Audor Pharma	Progesterone, micronized	APC01-141212P	1
Caelo	Progesterone, micronized	14253915	1
Euro OTC	Progesterone, micronized	141104301	1
Fagron	Progesterone, micronized	HTT140207	1
Caelo	Progesterone, micronized	12195924	2
Caelo	Progesterone, micronized	14K11-B04-300920	1
Caelo	Progesterone, micronized	14253929	1
Fagron	Progesterone, micronized	14K11-B04	3
Caelo	Progesterone, micronized	14H13-B05-3002016	1
Euro OTC	Progesterone, micronized	1503012-01	5
Audor Pharma	Progesterone, micronized	APC01-150311P	1
Fagron	Progesterone, micronized	14L15-B05-302292	2
Anzag	Progesterone, micronized	14k11-b04-300921	1
Fagron	Progesterone, micronized	14k11-b04	1
Fagron	Progesterone, micronized	13k28-b30-288261	1
Euro OTC	Progesterone, micronized	1506033-01	8
Fagron	Progesterone, micronized	15C31-B06-309790	2
keine Angabe	Progesterone, micronized	1304040-01	1
Caelo	Progesterone, micronized	2006500002	1
Fagron	Progesterone, micronized	15C31-B06	1
Euro OTC	Progesterone, micronized	1509008-01	3
Caelo	Progesterone, micronized	15124910	3
Fagron	Progesterone, micronized	HTT150201	2
Fagron	Progesterone, micronized	14K11B04300920	1
Audor Pharma	Progesterone, micronized	APC01-150708P	3
Fagron	Progesterone, micronized	15B12-Bo4-304838	1
Europh-Jenne	Progesterone, micronized	1406022-01	1
Fagron	Progesterone, micronized	15C31-B06-308439	7
Euro OTC	Progesterone, micronized	1509008-02	1
Euro	Progesterone, micronized	1509008-02	1
Fagron	Progesterone, micronized	15C31-B06-308796	2
sanacorp	Progesterone, micronized	15124902	1
Fagron	Progesterone, micronized	14K11-B04300921	1
Fagron	Progesterone, micronized	15C31-Bo6-308796	1
Caelo	Progesterone, micronized	15319603	42
Fagron	Progesterone, micronized	HTT140413	1
Euro OTC	Progesterone, micronized	150900801	1
Fagron	Progesterone, micronized	15C31B06308439	1
Anzag	Progesterone, micronized	15C31-B06-312963	3
Caelo	Progesterone, micronized	15319601	5
Anzag 07.04.2016	Progesterone, micronized	APC01-150708P	1
Caelo	Progesterone, micronized	1511-B05-313598	1
Caelo	Progesterone, micronized	15I11-B05-314184	2
Caelo	Progesterone, micronized	15C31-808	1
Fagron	Progesterone, micronized		2
Audor Pharma	Progesterone, micronized	APC01-151114P	3

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Supplier	Substance	Batch	Spectra
Euro OTC	Progesterone, micronized	1601009-01	8
Caelo	Progesterone, micronized	15319602	1
Caelo	Progesterone, micronized	4814A-03235	1
Fagron	Progesterone, micronized	15B12-B04-304837	2
Euro OTC	Progesterone, micronized	12195924	1
Fagron	Progesterone, micronized	15I11-B05-314842	1
Fagron	Progesterone, micronized	15C31-B06-313599	1
Caelo	Progesterone, micronized	16103603	11
Alliance	Progesterone, micronized	15i11-b05-315224	1
Fagron	Progesterone, micronized	16A20-B02-318667	3
Fagron	Progesterone, micronized	15I11-B05-314184	4
Ebert u. Jacobi 16.0...	Progesterone, micronized	15C31-B06-312963	1
Fagron	Progesterone, micronized	15C31-B06-312963	1
Phönix	Progesterone, micronized	15319604	1
Caelo	Progesterone, micronized	160100902	1
Caelo	Progesterone, micronized	15124919	1
Caelo	Progesterone, micronized	16A20-B02-319103	1
Caelo	Progesterone, micronized	161036303	9
Audor Pharma	Progesterone, micronized	APC01-160201P	2
Alliance	Progesterone, micronized	15I11-B05-315224	2
Caelo	Progesterone, micronized	15124902	1
Fagron	Progesterone, micronized	15C31-B06-316105	3
Euro OTC	Progesterone, micronized	1601009-02	4
Sanacorp	Progesterone, micronized	15/11-B05-315224	3
Phönix	Progesterone, micronized	16A20-B02-319103	1
Sanacorp	Progesterone, micronized	14C10-B01-293478	1
Audor Pharma	Progesterone, micronized	APC01-160201	1
Fagron	Progesterone, micronized	16A20-B02-321375	2
Fagron	Progesterone, micronized	15I11-B05	1
Fagron	Progesterone, micronized	15I1-B05-314184	1
Caelo	Progesterone, micronized	16103609	30
Caesar u Loretz	Progesterone, micronized	15124919	1
Fagron	Progesterone, micronized	15I11-B05-315224	1
Fagron	Progesterone, micronized	16A20-B02-321373	2
Fagron	Progesterone, micronized	16A20-B02-321374	4
Fagron	Progesterone, micronized	14K11-B04-300921	1
Fagron	Progesterone, micronized	15/11-B05-315224	2
Caelo	Progesterone, micronized	15319607	1
Fagron	Progesterone, micronized	1511-805	1
Fagron	Progesterone, micronized	16a20-b02-321375	1
Euro OTC	Progesterone, micronized	HTT160102	1
Caelo	Progesterone, micronized	16103601	2
Fagron	Progesterone, micronized	16a20-b02-318667	1
Caelo	Progesterone, micronized	16D13-B04	1
Caelo	Progesterone, micronized	15319608	6
Euro OTC	Progesterone, micronized	1605013-01	9
Fagron	Progesterone, micronized	16G15-B04-325279	3
Euro OTC	Progesterone, micronized	160100901	1
Caelo	Progesterone, micronized	15319618	2
Fagron	Progesterone, micronized	16G15-B04-325755	1
Caelo	Progesterone, micronized	16103613	20
Caelo	Progesterone, micronized	16103610	4
Fagron	Progesterone, micronized	15I11-B05-313598	1
Caelo	Progesterone, micronized	16015B14-315279	1
Caelo	Progesterone, micronized	16103602	2
Caelo	Progesterone, micronized	16103606	8
Fagron	Progesterone, micronized	16G15-B04-326487	3
Fagron	Progesterone, micronized	16G15-B04-32579	1
Fagron	Progesterone, micronized	16G15-B04-325135	1
Fagron	Progesterone, micronized	16g115-b04-325136	1

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Supplier	Substance	Batch	Spectra
Caelo	Progesterone, micronized	16103604	1
Caelo	Progesterone, micronized	15319619	1
Fagron	Progesterone, micronized	16G15-B04325136	1
Caelo	Progesterone, micronized	17060901	41
Phönix	Progesterone, micronized	1605013-01	1
Fagron	Progesterone, micronized	20170427Ma6	1
Fagron	Progesterone, micronized	16G15B04-325279	1
Fagron	Progesterone, micronized	16g15-b04	1
Fagron	Progesterone, micronized	EU-HTT160705	2
Euro OTC	Progesterone, micronized	1605013-02	8
Fagron	Progesterone, micronized	16J05-B04-328303	1
Fagron	Progesterone, micronized	16G15-B04-325136	3
Caelo	Progesterone, micronized	16L29-B03-330995	1
Fagron	Progesterone, micronized	16G15-B04	1
phönix	Progesterone, micronized	16g15-b04-326487	1
Ebert-Jacobi	Progesterone, micronized	16J05-B04-328263	1
Fagron	Progesterone, micronized	16L29-B03	1
Caesar&Lorenz	Progesterone, micronized	16103605	1
Fagron	Progesterone, micronized	16L29-B03-330995	1
Fagron	Progesterone, micronized	375779	1
Caelo	Progesterone, micronized	16103607	1
Caelo	Progesterone, micronized	1605013-02	1
Fagron	Progesterone, micronized	200650-0004	2
Caelo	Progesterone, micronized	EU-HTT160708	1
Fagron	Progesterone, micronized	17C15-B03-333672	2
Fagron	Progesterone, micronized	17C15-B03-333671	1
Fagron	Progesterone, micronized	16129b03332060	1
Fagron	Progesterone, micronized	16L29-B03-332060	4
Fagron	Progesterone, micronized	16J05-B04-328263	1
Fagron	Progesterone, micronized	16L29-B03-302060	1
Fagron	Progesterone, micronized	17C15-B03-333671	2
Fagron	Progesterone, micronized	17D25-B06-339655	2
Caelo	Progesterone, micronized	17060907	10
Fagron	Progesterone, micronized	16L29-B-332061	1
Caelo	Progesterone, micronized	B03333671	1
Caelo	Progesterone, micronized	17149903	1
Caelo	Progesterone, micronized	17060903	3
Euro OTC	Progesterone, micronized	1705028-01	5
Caelo	Progesterone, micronized	16103605	1
Euro OTC	Progesterone, micronized	1709012-01	3
Caerlo/Gehe	Progesterone, micronized	17060903	2
Sanacorp	Progesterone, micronized	17D25-B06	1
Cealo/Noweda	Progesterone, micronized	16103607	1
Euro OTC	Progesterone, micronized	160501303	2
Euro OTC	Progesterone, micronized	1605013-03	2
Caelo	Progesterone, micronized	1760911	1
Fagron	Progesterone, micronized	17D25-B06-339651	1
Caelo	Progesterone, micronized	1706093	1
Euro OTC	Progesterone, micronized	170502801	1
Caelo	Progesterone, micronized	15319620	1
Fagron	Progesterone, micronized	1605013-03	1
Fagron	Progesterone, micronized	17/21-B03-341517	1
Phoenix/Cealo	Progesterone, micronized	17/21-B03-341517	1
Fagron	Progesterone, micronized	17/21-B03-341518	1
Euro OTC	Progesterone, micronized	1801036-01	6
Audor Pharma	Progesterone, micronized	APC01-171101P	31
Caelo	Progesterone, micronized	1721bo3342134	1
Caelo	Progesterone, micronized	17060909	1
Fagron	Progesterone, micronized	17I21-B03-343284	1
Fagron	Progesterone, micronized	17I21-B03-342135	1

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Supplier	Substance	Batch	Spectra
Fagron	Progesterone, micronized	1511-B05-314842	1
Audor Pharma	Progesterone, micronized	APC01-170828P	1
Fagron	Progesterone, micronized	17I21-B03	1
Euro OTC	Progesterone, micronized	1705028	1
Fagron	Progesterone, micronized	17I08-B04	1
Euro OTC	Progesterone, micronized	17I08-B04	1
Fagron	Progesterone, micronized	intern20180619Ma3	1
Caelo	Progesterone, micronized	17/21-B03-343284	1
Fagron	Progesterone, micronized	17/21-B03-342135	2
Caelo	Progesterone, micronized	17060904	1
Fagron	Progesterone, micronized	17I08-B04-344773	1
Fagron	Progesterone, micronized	ApC01-180128P	1
Caelo	Progesterone, micronized	17348404	4
Fagron	Progesterone, micronized	18B06-B10-346701	1
Fagron	Progesterone, micronized	17/21-B03-343284	1
Fagron	Progesterone, micronized	C01-170814	1
Fagron	Progesterone, micronized	18B06-B10-347484	4
Audor Pharma	Progesterone, micronized	C01-180128	10
Audor Pharma	Progesterone, micronized	APC01-180610P	10
Fagron	Progesterone, micronized	18806-B10-349153	1
Euro OTC	Progesterone, micronized	1809017-01	1
Audor Pharma	Progesterone, micronized	APC01-181003P	10
Fagron	Progesterone, micronized	18F22-B04-353582	1
Fagron	Progesterone, micronized	18F22-B04353582-P201	1
Sanacorp	Progesterone, micronized	1809017-01	1

- 78 147 spectra from 565 *Apo-Ident* customers from a total of 25 872 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Progesterone, micronized* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Progesterone, micronized* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	440	0	74 056
Type B	0	2089	0	124 803
Type C	0	772	10	78 147

The substance/substance group *Progesterone, micronized* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 99.7128 %)
Type C	100.0000 % (> 99.8817 %)	98.7212 % (> 98.3376 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22525	22525	0.00	22.20
22226	22226	0.00	12.32
20718	22303	2.86	16.64
22301	22301	0.00	17.73
22303	22303	0.00	14.91
21868	21868	0.00	12.91
21870	21870	0.00	15.20
22830	21907	2.50	24.50
22831	22301	2.55	19.51
21907	21907	0.00	18.79

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Promethazine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20208-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Promethazine hydrochloride; Promethazini hydrochloridum

Special notes

When selecting the *Promethazine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Promethazine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Promethazine hyd...	13119214	21690	40	20130506
Caelo	Promethazine hyd...	161466	22628	40	20160621*
Caelo	Promethazine hyd...	17058601	23248	40	20170310

Validation samples

A total of 280 317 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 *Promethazine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Promethazine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Promethazine hydrochloride	13119214	21690 [†]	20
Caelo	Promethazine hydrochloride	170586	23324	40

- 126 832 spectra from a total of 2787 batches from further 781 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 *Promethazine hydrochloride*.

*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	Promethazine hydrochloride	11352305	1
Caelo	Promethazine hydrochloride	17058601	1
Caelo	Promethazine hydrochloride	13119211	1
Caelo	Promethazine hydrochloride	19051805	1

- 78 925 spectra from 565 *Apo-Ident* customers from a total of 26 133 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Promethazine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Promethazine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	60	0	126 832
Type C	0	3	1	78 925

The substance/substance group *Promethazine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.8820 %)	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
21690	22628	2.38	63.85
22628	22628	0.00	65.82
23248	22628	4.67	63.18

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Propranolol hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20954-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Propranolol hydrochloride; Propranololi hydrochloridum

Special notes

When selecting the *Propranolol hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Propranolol hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Propranolol hydr...	13I13-N04	20954	40	1402307
Caelo	Propranolol hydr...	12370712	21396	40	20130116
Caelo	Propranolol hydr...	12370712	21410	40	20130116
Fagron	Propranolol hydr...	15F16-B02-312979	22591	40	20150630

Validation samples

A total of 280317 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 *Propranolol hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1620 batches from further 372 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 *Propranolol hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propranolol hydrochloride	12370712	21396 [†]	20
Caelo	Propranolol hydrochloride	12370712	21410 [†]	20
Caelo	Propranolol hydrochloride	15283302	22590	40
Caelo	Propranolol hydrochloride	171722	23650	40
Caelo	Propranolol hydrochloride	173330	23836	40

- 126732 spectra from a total of 2785 batches from further 781 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.

- 288 spectra from 170 *Apo-Ident* customers from 100 batches from the substance/substance group *Propranolol hydrochloride*.

[†]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
Fagron	Propranolol hydrochloride	11L01-N05	2
Caelo	Propranolol hydrochloride	12a27-n04	1
Fagron	Propranolol hydrochloride	12D27-N14	4
Fagron	Propranolol hydrochloride	31101201	1
Fagron	Propranolol hydrochloride	12A27-N04	1
InfectoPharm	Propranolol hydrochloride	J0512011	1
Gehe	Propranolol hydrochloride		1
Caelo	Propranolol hydrochloride	12D27-N14	1
Fagron	Propranolol hydrochloride	20250711-8	1
Löwen City-Apotheke Bar...	Propranolol hydrochloride	4012013	1
Fagron	Propranolol hydrochloride	12F29-N06	4
Fagron	Propranolol hydrochloride	402310015	1
Fagron	Propranolol hydrochloride	12F29-N06	1
Fagron	Propranolol hydrochloride	12K06-N07	7
Fargon	Propranolol hydrochloride	12K06-N07	1
Fagron	Propranolol hydrochloride	11I19-N09	1
Caelo	Propranolol hydrochloride	12370703	1
Noweda	Propranolol hydrochloride		1
Fagron	Propranolol hydrochloride	1313-N04	2
Fagron	Propranolol hydrochloride	12K06N07	1
Fagron	Propranolol hydrochloride	9L09-N06	1
fragon/AHD	Propranolol hydrochloride	13/13-N04	1
Fagron	Propranolol hydrochloride	3050PRRII	2
Fagron	Propranolol hydrochloride	13I13-N04	7
Fagron	Propranolol hydrochloride	13/13-N04	4
Caelo	Propranolol hydrochloride	13/13-N04	3
Fagron	Propranolol hydrochloride	9CMK6AA71374	1
Fagron	Propranolol hydrochloride		1
Fagron	Propranolol hydrochloride	13J13-N04	3
Gutenberg-Apotheke	Propranolol hydrochloride	13I13-N04	1
Fagron	Propranolol hydrochloride	11D01-N11	1
Caelo	Propranolol hydrochloride	M130104	1
Caelo	Propranolol hydrochloride	12370710	1
Sanacorp	Propranolol hydrochloride	12370712	1
Fagron	Propranolol hydrochloride	13E15-B40-289355	11
Fagron	Propranolol hydrochloride	4071401	1
Fagron	Propranolol hydrochloride	3112U-03609	1
Fagron	Propranolol hydrochloride	13113-N04	1
Fagron	Propranolol hydrochloride	3050PRII	1
Fagron	Propranolol hydrochloride	13E15-B40	5
Fagron	Propranolol hydrochloride	3913M-03609	1
Caelo	Propranolol hydrochloride	12370709	1
Caelo	Propranolol hydrochloride	13I13N04	1
Fagron	Propranolol hydrochloride	5101	1
Caelo	Propranolol hydrochloride	m130104	1
Fagron	Propranolol hydrochloride	13E15-B40-294297	5
Caelo	Propranolol hydrochloride	12370712	1
Caelo	Propranolol hydrochloride	13E15-B40-289355	1
Caelo	Propranolol hydrochloride	13379804	1
Euro OTC	Propranolol hydrochloride	13379806	1
Euro OTC	Propranolol hydrochloride	13I13-N04	1
Caelo	Propranolol hydrochloride	13379806	1
Alliance health	Propranolol hydrochloride	13E15-B40-294297	1
phönix	Propranolol hydrochloride	2/AKD3	1
Caelo	Propranolol hydrochloride	13379807	4
Caesar u Loretz	Propranolol hydrochloride	13379807	1
Fagron	Propranolol hydrochloride	13E15-B40-297021	6
Caelo	Propranolol hydrochloride	13379809	3
Fagron	Propranolol hydrochloride	28051508	1
Gehe Kassel 26.06.2015	Propranolol hydrochloride	15082401	1

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Supplier	Substance	Batch	Spectra
Fagron	Propranolol hydrochloride	13E15B40-297021	1
Caelo	Propranolol hydrochloride	15082401	4
Calo/AHD	Propranolol hydrochloride	15082401	1
Caelo	Propranolol hydrochloride	15082404	1
Inresa 22.09.15	Propranolol hydrochloride	3043PRRII	1
Caelo	Propranolol hydrochloride	15082405	2
Fagron	Propranolol hydrochloride	M130104	1
Caelo	Propranolol hydrochloride	15283301	10
Caelo	Propranolol hydrochloride	15F16-B02-312979	3
Caelo	Propranolol hydrochloride	15F16-B02	1
Caelo	Propranolol hydrochloride	15283302	5
Fagron	Propranolol hydrochloride	15F16B02312979	1
Fagron	Propranolol hydrochloride	15F16-B02-312979	2
Changzhou Yabang Pharma...	Propranolol hydrochloride	15F16-B02	1
Fagron	Propranolol hydrochloride	15K11-B01-316401	9
Caelo/Noweda	Propranolol hydrochloride	15283302	1
Caelo	Propranolol hydrochloride	1542251	1
Fagron	Propranolol hydrochloride	15K11-Bo1-316401	1
Fagron	Propranolol hydrochloride	15K11-B01	2
Caelo	Propranolol hydrochloride	15422501	9
allianz	Propranolol hydrochloride	15283302	1
Caelo	Propranolol hydrochloride	15K11-B01-316401	1
Caelo	Propranolol hydrochloride	15422502	11
Caelo	Propranolol hydrochloride	154225	1
Fagron	Propranolol hydrochloride	15K11-B01-320607	6
WE:Phönix 12.08.2016	Propranolol hydrochloride	15422502	1
Caelo	Propranolol hydrochloride	15422505	6
Caelo	Propranolol hydrochloride	M141203	1
Audor Pharma	Propranolol hydrochloride	15K11-B01	1
Caelo	Propranolol hydrochloride	15k11-B01	1
Caelo	Propranolol hydrochloride	16138302	5
Fagron	Propranolol hydrochloride	15K11-B01-322717	2
Phönix	Propranolol hydrochloride	15k11-b01-322717	1
Noweda/Apomix	Propranolol hydrochloride	15K11-B01-316401	1
Fagron	Propranolol hydrochloride	16138302	1
Euro OTC	Propranolol hydrochloride	16138304	2
Fagron	Propranolol hydrochloride	16E09-B09-326637	5
Fagron	Propranolol hydrochloride	700556-0001	1
Fagron	Propranolol hydrochloride	M141203	1
Caelo	Propranolol hydrochloride	16E09-B09-326637	1
phönix	Propranolol hydrochloride	16e09b09326637	1
/O. Geilenkirchen	Propranolol hydrochloride	15422502	1
Fagron	Propranolol hydrochloride	15F16-B02	1
Caelo	Propranolol hydrochloride	16138304	5
Gehe	Propranolol hydrochloride	16E09-B09	1
phönix	Propranolol hydrochloride	16e09-b09	1
Fagron	Propranolol hydrochloride	16E09-B09	1
Fagron	Propranolol hydrochloride	16E09-B09-330547	3
Sanacorp	Propranolol hydrochloride	16138304	1
AHD	Propranolol hydrochloride	941895	1
Fagron	Propranolol hydrochloride	16E09-B09333442	1
Caelo	Propranolol hydrochloride	150082405	1
Fagron	Propranolol hydrochloride	16E09-B09-333442	3
Caelo	Propranolol hydrochloride	17172203	5
Phoenix/Fargron	Propranolol hydrochloride	15K11-B01-322717	2
Caelo	Propranolol hydrochloride	17172204	7
AHD	Propranolol hydrochloride	17172204	2
Fagron	Propranolol hydrochloride	17K22-B03-342731	4
Caelo	Propranolol hydrochloride	17172205	1
Caelo	Propranolol hydrochloride	1712204	1

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Supplier	Substance	Batch	Spectra
Fagron	Propranolol hydrochloride	18041807	1
Caelo	Propranolol hydrochloride	17333001	6
Caelo	Propranolol hydrochloride	17333005	1
Caelo	Propranolol hydrochloride	17K22-B03-344247	1
AHD	Propranolol hydrochloride	17333001	1
Jenne	Propranolol hydrochloride	17333001	1
Caelo	Propranolol hydrochloride	1733301	1
Fagron	Propranolol hydrochloride	17K-22-B03-345013	1
Caelo	Propranolol hydrochloride	173330015654	1
Fagron	Propranolol hydrochloride	17K22-B03-350048	1
Caelo	Propranolol hydrochloride	17333006	2
Caelo	Propranolol hydrochloride	18179402	3
Caelo	Propranolol hydrochloride	17K22-B03-347251	1
Sanacorp	Propranolol hydrochloride	18D23-B09-351774	1

- 78 641 spectra from 565 *Apo-Ident* customers from a total of 26 037 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Propranolol hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Propranolol hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	160	0	126 732
Type C	0	211	77	78 641

The substance/substance group *Propranolol hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	73.2639 % (> 72.2222 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20954	20954	0.00	54.42
21396	20954	2.11	54.29
21410	20954	12.24	53.41
22591	20954	9.27	54.72

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Propyl-4-hydroxybenzoate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20981-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Propyl-4-hydroxybenzoate; Propylis parahydroxybenzoas

Special notes

When selecting the *Propyl-4-hydroxybenzoate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Propyl-4-hydroxybenzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propyl-4-hydroxy...	11373523	20981	40	1402440
Caelo	Propyl-4-hydroxy...	13365009	21758	40	20131203
Caelo	Propyl-4-hydroxy...	162595	22754	40	20161005*

Validation samples

A total of 280 317 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 *Propyl-4-hydroxybenzoate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Propyl-4-hydroxybenzoate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propyl-4-hydroxybenzoate	13365009	21758 [†]	20
Caelo	Propyl-4-hydroxybenzoate	162595	22765	40
Caelo	Propyl-4-hydroxybenzoate	171970	23675	40

- 126 792 spectra from a total of 2786 batches from further 781 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.

- 128 spectra from 88 *Apo-Ident* customers from 50 batches from the substance/substance group *Propyl-4-hydroxybenzoate*.

*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	Propyl-4-hydroxybenzoate	11373505	1
Caelo	Propyl-4-hydroxybenzoate	1108211931	1
Anzag	Propyl-4-hydroxybenzoate	11373512	2
Caelo	Propyl-4-hydroxybenzoate	11102624	1
Caelo	Propyl-4-hydroxybenzoate	11373512	3
Caelo	Propyl-4-hydroxybenzoate	11102611	2
Fagron	Propyl-4-hydroxybenzoate	610M-01931	1
Caelo	Propyl-4-hydroxybenzoate	713Q-01931	1
Caelo	Propyl-4-hydroxybenzoate	11102609	1
Caelo	Propyl-4-hydroxybenzoate	11373518	2
Fagron	Propyl-4-hydroxybenzoate	12B13-N04	1
Noweda	Propyl-4-hydroxybenzoate	11373505	1
Caelo	Propyl-4-hydroxybenzoate	113735223	1
Caesar/Noweda	Propyl-4-hydroxybenzoate	3710M-01931	2
AHD	Propyl-4-hydroxybenzoate	11373523	1
Euro OTC	Propyl-4-hydroxybenzoate	2509025	1
Caelo	Propyl-4-hydroxybenzoate	11373523	2
Caelo	Propyl-4-hydroxybenzoate	11373524	1
Caelo	Propyl-4-hydroxybenzoate	290114PML03	1
Caelo	Propyl-4-hydroxybenzoate	13100215	7
Phönix 14.01.2014	Propyl-4-hydroxybenzoate	11373526	1
Caelo	Propyl-4-hydroxybenzoate	82792159	1
Gehe 5.3.14	Propyl-4-hydroxybenzoate	13100215	1
Caelo	Propyl-4-hydroxybenzoate	3041408	1
PHOENIX 10.03.2014	Propyl-4-hydroxybenzoate	11373526	1
siehe WE-Prüfprotokoll	Propyl-4-hydroxybenzoate	84/11	1
Phoenix	Propyl-4-hydroxybenzoate	13100215	1
Caesar &Loretz GmbH	Propyl-4-hydroxybenzoate	13100215	1
Caelo	Propyl-4-hydroxybenzoate	13100217	2
Caelo	Propyl-4-hydroxybenzoate	13100218	2
Caelo	Propyl-4-hydroxybenzoate	13100208	1
Caelo	Propyl-4-hydroxybenzoate	1913I-01931	1
Caelo	Propyl-4-hydroxybenzoate	221014PAS01	1
GATT-KOLLER/PHOENIX	Propyl-4-hydroxybenzoate	5080/11130214	1
Caelo	Propyl-4-hydroxybenzoate	13365006	5
Sanacorp	Propyl-4-hydroxybenzoate	AKD3	1
Caelo	Propyl-4-hydroxybenzoate	13365009	3
Caelo	Propyl-4-hydroxybenzoate	13365011	5
Caelo	Propyl-4-hydroxybenzoate	13051504	1
Caelo	Propyl-4-hydroxybenzoate	13365012	2
Caelo	Propyl-4-hydroxybenzoate	13100219	1
Caelo	Propyl-4-hydroxybenzoate	4314U-01931	1
Caelo	Propyl-4-hydroxybenzoate	14359009	1
Caelo	Propyl-4-hydroxybenzoate	14359008	19
Caelo	Propyl-4-hydroxybenzoate	14359005	8
Caelo	Propyl-4-hydroxybenzoate	14359006	3
Noweda	Propyl-4-hydroxybenzoate	14359005	1
Caelo	Propyl-4-hydroxybenzoate	15246501	1
Caelo	Propyl-4-hydroxybenzoate	3115M-01931	1
Caelo	Propyl-4-hydroxybenzoate	14359019	1
Caelo	Propyl-4-hydroxybenzoate	15246502	2
Caelo	Propyl-4-hydroxybenzoate	14359020	4
Caelo	Propyl-4-hydroxybenzoate	16359006	1
Noweda	Propyl-4-hydroxybenzoate	14359020	1
Caelo	Propyl-4-hydroxybenzoate	16259505	5
Caelo	Propyl-4-hydroxybenzoate	15276514	1
Caelo	Propyl-4-hydroxybenzoate	16259516	8
Sanacorp	Propyl-4-hydroxybenzoate	16259516	1
Caelo	Propyl-4-hydroxybenzoate	11121709	1
Caelo	Propyl-4-hydroxybenzoate	17343108	1

- 78 801 spectra from 565 *Apo-Ident* customers from a total of 26 089 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Propyl-4-hydroxybenzoate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Propyl-4-hydroxybenzoate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	98	30	78 801

The substance/substance group *Propyl-4-hydroxybenzoate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	76.5625 % (> 74.2188 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21758	22754	6.28	20.23
22754	22754	0.00	18.60
20981	20981	0.00	23.86

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Propyphenazone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20805-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Propyphenazone; Propyphenazonum

Special notes

When selecting the *Propyphenazone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Propyphenazone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propyphenazone	12039103	20805	40	1402051
Caelo	Propyphenazone	13332206	21454	40	20131009
Fagron	Propyphenazone	16E02-B08-327928	23261	40	20160602
Fagron	Propyphenazone	16H25-B01-334972	23922	40	20161227

Validation samples

A total of 280317 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 *Propyphenazone*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 *Propyphenazone*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propyphenazone	13332206	21454 [†]	20
Caelo	Propyphenazone	15348908	23254	40
Caelo	Propyphenazone	172776	23861	40

- 126792 spectra from a total of 2786 batches from further 781 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 8 *Apo-Ident* customers from 24 batches from the substance/substance group *Propyphenazone*.

[†]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	Propyphenazone		1
Fargon	Propyphenazone	11H31-N07	1
Caelo	Propyphenazone	12039101	2
Caelo	Propyphenazone	12039103	1
Caelo	Propyphenazone	12039112	1
Caelo	Propyphenazone	13036702	2
Caelo	Propyphenazone	13332205	3
Gatt-Koller / Phoenix	Propyphenazone	419/02123112	1
Raben-Apotheke Mildenau	Propyphenazone	12039103	1
Fargon	Propyphenazone	13B12-B02-297171	1
Caelo	Propyphenazone	13137104	1
Fargon	Propyphenazone	13K20-B03	2
Caelo	Propyphenazone	15122502	1
Caelo	Propyphenazone	15122505	1
Fargon	Propyphenazone	13K20-B03-311715	3
Caelo	Propyphenazone	15122504	2
Fargon	Propyphenazone	13K-B03-319137	1
Caelo	Propyphenazone	15348902	1
Fargon	Propyphenazone	13K20B03319137	1
Fargon	Propyphenazone	13k20-b03-319137	1
Fargon	Propyphenazone	13K20-B03-319137	3
Caelo	Propyphenazone	15348904	2
Fargon	Propyphenazone	16E02-B08-327928	2
Caelo	Propyphenazone	15348912	2
Caelo	Propyphenazone	17351305	1

- 78 891 spectra from 565 *Apo-Ident* customers from a total of 26 113 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Propyphenazone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Propyphenazone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	100	0	126 792
Type C	0	34	4	78 891

The substance/substance group *Propyphenazone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	89.4737 % (> 81.5789 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
23922	20805	7.35	45.68
20805	20805	0.00	46.21
21454	20805	3.57	46.13
23261	20805	5.37	46.47

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Pyridoxal-5-phosphate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20830-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Pyridoxal-5-phosphate; Pyridoxali phosphas

Special notes

When selecting the *Pyridoxal-5-phosphate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Pyridoxal-5-phosphate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Pyridoxal-5-phos...	1302029-01	20830	40	8897
Euro OTC	Pyridoxal-5-phos...	1701015	23133	40	20170220*
Euro OTC	Pyridoxal-5-phos...	1711030	23877	40	20171215*
Euro OTC	Pyridoxal-5-phos...	1808030	24329	40	20181019*

Validation samples

A total of 280 317 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 *Pyridoxal-5-phosphate*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Pyridoxal-5-phosphate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Pyridoxal-5-phosphate	1302029-01	21097	40
Euro OTC	Pyridoxal-5-phosphate	1701015-01	23276	40

- 126 812 spectra from a total of 2787 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 7 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Pyridoxal-5-phosphate*.

*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
Denk	Pyridoxal-5-phosphate	C041402802	1
Euro OTC	Pyridoxal-5-phosphate	1701015-01	3
Inresa Arznei	Pyridoxal-5-phosphate	13100411	1
Denk	Pyridoxal-5-phosphate	20171202	1
Euro OTC	Pyridoxal-5-phosphate	1711030-01	1

- 78 922 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Pyridoxal-5-phosphate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pyridoxal-5-phosphate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	113	47	74 336
Type B	0	80	0	126 812
Type C	0	7	0	78 922

The substance/substance group *Pyridoxal-5-phosphate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	70.6250 % (> 68.7500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8818 %)	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
20830	20830	0.00	47.38
23133	23133	0.00	50.95
24329	24329	0.00	57.34
23877	23877	0.00	54.86

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Pyridoxine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20440-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Pyridoxine hydrochloride; Pyridoxini hydrochloridum

Special notes

When selecting the *Pyridoxine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Pyridoxine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pyridoxine hydro...	14262302	21675	40	20141002
Euro OTC	Pyridoxine hydro...	1401044-01	21678	40	20140221
Euro OTC	Pyridoxine hydro...	1407009-01	21773	40	20140807
Euro OTC	Pyridoxine hydro...	1507012	21846	40	20150721*
Euro OTC	Pyridoxine hydro...	1601039	22300	40	20160203*

Validation samples

A total of 280 317 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 *Pyridoxine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1618 batches from further 372 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 *Pyridoxine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pyridoxine hydrochloride	14262302	21675 [†]	20
Euro OTC	Pyridoxine hydrochloride	1401044-01	21678 [†]	20
Euro OTC	Pyridoxine hydrochloride	1407009-01	21773 [†]	20
Euro OTC	Pyridoxine hydrochloride	1507012	21846 [†]	20
Euro OTC	Pyridoxine hydrochloride	1601039	22300 [†]	20
Euro OTC	Pyridoxine hydrochloride	1604063	22569	40
Caelo	Pyridoxine hydrochloride	162225	22770	40
Euro OTC	Pyridoxine hydrochloride	1608035	22798	40
Euro OTC	Pyridoxine hydrochloride	1710014	23735	40
Caelo	Pyridoxine hydrochloride	180287	24024	40
Euro OTC	Pyridoxine hydrochloride	1806022-01	24189	40

- 126 552 spectra from a total of 2778 batches from further 781 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.

- 68 spectra from 13 *Apo-Ident* customers from 29 batches from the substance/substance group *Pyridoxine hydrochloride*.

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH D-...	Pyridoxine hydrochloride	11197009	5
Caesar & Loretz GmbH, 4...	Pyridoxine hydrochloride	12214102	5
Caesar & Loretz GmbH, 4...	Pyridoxine hydrochloride	12214110	2
Caesar & Loretz GmbH, 4...	Pyridoxine hydrochloride	12214115	7
Caelo	Pyridoxine hydrochloride	11197009	1
Caelo	Pyridoxine hydrochloride	12214102	2
Caesar & Loretz GmbH, 4...	Pyridoxine hydrochloride	12214119	2
Fagron	Pyridoxine hydrochloride	12e02-n02	1
Euro OTC	Pyridoxine hydrochloride	1206022-02	1
Caelo	Pyridoxine hydrochloride	11021406	1
Fagron	Pyridoxine hydrochloride	L13080030	1
Caelo	Pyridoxine hydrochloride	12214119	2
Caelo	Pyridoxine hydrochloride	13102510	2
Euro OTC	Pyridoxine hydrochloride	1110001-01	1
Caelo	Pyridoxine hydrochloride	13102509	2
Caelo	Pyridoxine hydrochloride	13102516	1
Caelo	Pyridoxine hydrochloride	12102510	1
Caelo	Pyridoxine hydrochloride	14262302	3
Caelo	Pyridoxine hydrochloride	14262306	1
Caelo	Pyridoxine hydrochloride	15218702	6
Euro OTC	Pyridoxine hydrochloride	1601039-01	1
Caelo	Pyridoxine hydrochloride	15218713	3
Caelo	Pyridoxine hydrochloride	15218707	1
Caelo	Pyridoxine hydrochloride	15218710	2
Euro OTC	Pyridoxine hydrochloride	1604063-01	1
Caelo	Pyridoxine hydrochloride	15218709	1
Caelo	Pyridoxine hydrochloride	16222501	5
Caelo	Pyridoxine hydrochloride	16222514	2
Farmalabor	Pyridoxine hydrochloride	P1701531-000	1
Caelo	Pyridoxine hydrochloride	16222521	1
Caelo	Pyridoxine hydrochloride	16222506	1
Caelo	Pyridoxine hydrochloride	16222515	2

- 78 861 spectra from 565 *Apo-Ident* customers from a total of 26 108 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Pyridoxine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pyridoxine hydrochloride*

and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	340	0	126 552
Type C	0	66	2	78 861

The substance/substance group *Pyridoxine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.2353 %)
Type C	100.0000 % (> 99.8817 %)	97.0588 % (> 92.6471 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21675	21846	6.11	93.92
21678	21846	6.06	93.77
21773	21846	1.01	95.39
21846	21846	0.00	94.89
22300	22300	0.00	95.18

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Quinidine sulfate dihydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20819-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Quinidine sulfate dihydrate; Chinidini sulfas; Quinidine sulphate dihydrate

Special notes

When selecting the *Quinidine sulfate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Quinidine sulfate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Quinidine sulfat...	12L04-N10	20819	40	AR-14-FG-013249-01
Fagron	Quinidine sulfat...	12J16-B03	21217	39	1412323
Fagron	Quinidine sulfat...	14I04-B09-304357	21810	40	AR-15-FG-015409-01

Validation samples

A total of 280317 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 *Quinidine sulfate dihydrate*. These samples are listed above in the [calibration samples](#) section.
- 74377 spectra from a total of 1620 batches from further 372 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 *Quinidine sulfate dihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Quinidine sulfate dihydrate	14I04-B09-304357	21810 [†]	20
Fagron	Quinidine sulfate dihydrate	16A06-B04-324954	22970	40
Fagron	Quinidine sulfate dihydrate	18B01-B08-350965	24181	40

- 126792 spectra from a total of 2786 batches from further 781 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 *Quinidine sulfate dihydrate*.

Supplier	Substance	Batch	Spectra
Fagron	Quinidine sulfate dihydrate	13G08-N02	1
buchler GmbH	Quinidine sulfate dihydrate	16a06-b04-340797	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*.

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Quinidine sulfate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinidine sulfate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 377
Type B	0	100	0	126 792
Type C	0	2	0	78 927

The substance/substance group *Quinidine sulfate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 94.9580 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8823 %)	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
20819	20819	0.00	30.79
21217	21217	0.00	30.40
21810	21810	0.00	31.40

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Quinine dihydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	23186-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Quinine dihydrochloride; Chinini dihydrochloridum

Special notes

When selecting the *Quinine dihydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Quinine dihydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Quinine dihydroc...	172129	23636	40	20173008*
Caelo	Quinine dihydroc...	172072	23655	40	20170830*

Validation samples

A total of 280 317 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 *Quinine dihydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Quinine dihydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Quinine dihydrochloride	16269603	23185	40
Caelo	Quinine dihydrochloride	16269603	23186	40
Caelo	Quinine dihydrochloride	162696	23358	40

- 126 772 spectra from a total of 2787 batches from further 781 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 *Quinine dihydrochloride*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

*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.

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 *Quinine dihydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinine dihydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	120	0	126 772
Type C	0	0	0	78 929

The substance/substance group *Quinine dihydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
23636	23636	0.00	76.38
23655	23655	0.00	75.43

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Quinine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20547-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Quinine hydrochloride; Chinini hydrochloridum

Special notes

When selecting the *Quinine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Quinine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Quinine hydrochl...	13G10-N07	21235	30	20130809
Fagron	Quinine hydrochl...	13I30-B02-295630	21809	40	AR-15-FG-015410-01
Caelo	Quinine hydrochl...	15376201	22309	40	20151105
Caelo	Quinine hydrochl...	16283302	23577	40	1802260

Validation samples

A total of 280317 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 *Quinine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74346 spectra from a total of 1619 batches from further 372 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 *Quinine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Quinine hydrochloride	13I30-B02-295630	21809 [†]	20
Caelo	Quinine hydrochloride	15376201	22309 [†]	20
Fagron	Quinine hydrochloride	15A20-B03-319027	23573	40
Fagron	Quinine hydrochloride	16K01-B05-340171	23920	40
Caelo	Quinine hydrochloride	180226	24022	40

- 126732 spectra from a total of 2784 batches from further 781 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.

- 10 spectra from 10 *Apo-Ident* customers from 10 batches from the substance/substance group *Quinine hydrochloride*.

[†]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	Quinine hydrochloride	12316605	1
Caelo	Quinine hydrochloride	12316604	1
Fagron	Quinine hydrochloride	10N129B	1
Caelo	Quinine hydrochloride	13D24-N06	1
Gatt-Koller	Quinine hydrochloride	3500/08103810	1
Fagron	Quinine hydrochloride	13G10-N07	1
Caelo	Quinine hydrochloride	12316611	1
Caelo	Quinine hydrochloride	153776201	1
Caelo	Quinine hydrochloride	16283302	1
Caelo	Quinine hydrochloride	16283305	1

- 78 919 spectra from 565 *Apo-Ident* customers from a total of 26 127 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Quinine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 346
Type B	0	160	0	126 732
Type C	0	10	0	78 919

The substance/substance group *Quinine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8818 %)	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
21235	23577	8.17	42.51
21809	21809	0.00	24.53
22309	23577	1.51	33.91
23577	23577	0.00	33.97

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Quinine sulfate dihydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	21057-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Quinine sulfate dihydrate; Chinini sulfas; Quinine sulphate dihydrate

Special notes

When selecting the *Quinine sulfate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Quinine sulfate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Quinine sulfate ...	13J23-N03	21057	40	1404401
Fagron	Quinine sulfate ...	14B27-B01	21277	40	AR-16-FG-009455-01
Caelo	Quinine sulfate ...	13024604	21429	40	AR-16-FG-005472-01

Validation samples

A total of 280 317 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 *Quinine sulfate dihydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Quinine sulfate dihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Quinine sulfate dihydrate	13024604	21429 [†]	20
Caelo	Quinine sulfate dihydrate	15230005	22959	40
Caelo	Quinine sulfate dihydrate	170616	23281	40
Caelo	Quinine sulfate dihydrate	170616	23316	40
Caelo	Quinine sulfate dihydrate	180630	24032	40

- 126 712 spectra from a total of 2785 batches from further 781 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 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Quinine sulfate dihydrate*.

[†]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
Gatt-Koller / Phoenix	Quinine sulfate dihydrate	4928/11132214	1
Gatt-Koller / Phoenix	Quinine sulfate dihydrate	2503/07143314	1
Caelo	Quinine sulfate dihydrate	15B06B03304359	1

- 78 926 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Quinine sulfate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinine sulfate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	180	0	126 712
Type C	0	3	0	78 926

The substance/substance group *Quinine sulfate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8821 %)	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
21057	21057	0.00	11.77
21429	21429	0.00	11.62
21277	21277	0.00	12.58

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Quinoline yellow
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20456-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Quinoline yellow

Special notes

When selecting the *Quinoline yellow* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Quinoline yellow*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Quinoline yellow	12E24-N01	20731	40	20120601
Caelo	Quinoline yellow	12042010	20922	40	20120314
Caelo	Quinoline yellow	13109108	21305	40	1711481
Caelo	Quinoline yellow	17034101	23400	40	1709327

Validation samples

A total of 280317 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 *Quinoline yellow*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 *Quinoline yellow*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Quinoline yellow	12E24-N01	20731 [†]	20
Caelo	Quinoline yellow	16050101	23401	40
Caelo	Quinoline yellow	172277	23685	30

- 126802 spectra from a total of 2786 batches from further 781 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.

- 68 spectra from 41 *Apo-Ident* customers from 37 batches from the substance/substance group *Quinoline yellow*.

[†]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	Quinoline yellow	11089606	1
Fagron	Quinoline yellow	12B08-N08	1
Caelo	Quinoline yellow	713E-03146	1
Caelo	Quinoline yellow	20301211-6	1
Fagron	Quinoline yellow	9878	1
Caelo	Quinoline yellow	12042002	3
Fagron	Quinoline yellow	11F30-N04	1
Caelo	Quinoline yellow	11089608	1
Fagron	Quinoline yellow	11K08-N01	2
Caelo	Quinoline yellow	12042007	3
Fagron	Quinoline yellow	12E24-N05	1
Fagron	Quinoline yellow	12L11-N07	1
Caelo	Quinoline yellow	12042010	1
Fagron	Quinoline yellow	100427	1
PHOENIX	Quinoline yellow	12042004	1
Caelo	Quinoline yellow	13109102	2
sanacorp	Quinoline yellow	3214M-03146	1
Caelo	Quinoline yellow	14049401	2
Caelo	Quinoline yellow	13109109	1
Caelo	Quinoline yellow	14274309	1
Caelo	Quinoline yellow	11089610	1
Fagron	Quinoline yellow	14D18-B02-295783	1
Caelo	Quinoline yellow	14363202	3
Caelo	Quinoline yellow	14274305	1
Caelo	Quinoline yellow	15276803	2
Caelo	Quinoline yellow	14363207	1
Caelo	Quinoline yellow	15276802	1
phönix	Quinoline yellow	15276803	1
Caelo	Quinoline yellow	15276804	2
Caelo	Quinoline yellow	15276801	1
Caelo	Quinoline yellow	16050101	5
Caelo	Quinoline yellow	16050106	3
Caelo	Quinoline yellow	17034102	5
Caelo	Quinoline yellow	17034104	6
Caelo	Quinoline yellow	17034101	1
Caelo	Quinoline yellow	118E-03146	1
Caelo	Quinoline yellow	17227701	3
Caelo	Quinoline yellow	17227703	3

- 78 861 spectra from 565 *Apo-Ident* customers from a total of 26 100 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Quinoline yellow* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinoline yellow* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	63	27	126 802
Type C	0	38	30	78 861

The substance/substance group *Quinoline yellow* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	70.0000 % (> 66.6667 %)
Type C	100.0000 % (> 99.8817 %)	55.8824 % (> 51.4706 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20731	21305	25.52	77.11
20922	21305	9.43	81.95
21305	21305	0.00	94.30
23400	23400	0.00	57.84

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Quinolinol sulfate potassium sulfate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20573-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Quinolinol sulfate potassium sulfate; Chinolini et kalii sulfas; Quinolinol sulphate potassium sulphate

Special notes

When selecting the *Quinolinol sulfate potassium sulfate* substance/substance group, the following information is displayed to the user:

- Advice for the distinction from 8-hydroxyquinoline sulfate: 8-hydroxyquinoline sulfate is a spectrally similar substance, which is however currently not deliverable in Germany. Please decide, if an additional prove seems to be useful.

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Quinolinol sulfate potassium sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Quinolinol sulfa...	13071104	20983	40	1403095
Caelo	Quinolinol sulfa...	13403501	21430	40	20131218
Caelo	Quinolinol sulfa...	15147704	22606	40	20150618
Caelo	Quinolinol sulfa...	162218	22626	40	20160808*

Validation samples

A total of 280 317 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 *Quinolinol sulfate potassium sulfate*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Quinolinol sulfate potassium sulfate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Quinolinol sulfate potassium...	13403501	21430 [†]	20
Caelo	Quinolinol sulfate potassium...	15147704	22607	40
Caelo	Quinolinol sulfate potassium...	16221809	23563	40

- 126 792 spectra from a total of 2786 batches from further 781 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*.

- 182 spectra from 93 *Apo-Ident* customers from 22 batches from the substance/substance group *Quinolinol sulfate potassium sulfate*.

Supplier	Substance	Batch	Spectra
Stumpf	Quinolinol sulfate potassium...	100804	1
Dermapharm	Quinolinol sulfate potassium...	100804	11
Caelo	Quinolinol sulfate potassium...	10281601	1
Dermapharm	Quinolinol sulfate potassium...	120905	42
Caelo	Quinolinol sulfate potassium...	120905	1
Caelo	Quinolinol sulfate potassium...	7051305	1
Caelo	Quinolinol sulfate potassium...	9106304	1
Phönix Gotha	Quinolinol sulfate potassium...	120905	4
Nachprüfung	Quinolinol sulfate potassium...	2812U03423	1
Caelo	Quinolinol sulfate potassium...	13071101	2
Caelo	Quinolinol sulfate potassium...	13071104	5
Caelo	Quinolinol sulfate potassium...	13403501	6
Caelo	Quinolinol sulfate potassium...	13071106	1
sanacorp	Quinolinol sulfate potassium...	120905	1
Mibe	Quinolinol sulfate potassium...	120905	1
dermopharm/Noweda	Quinolinol sulfate potassium...	120905	1
Dermapharm	Quinolinol sulfate potassium...	140804	47
Caelo	Quinolinol sulfate potassium...	13403506	12
Dermäphärm	Quinolinol sulfate potassium...	140804	1
Caelo	Quinolinol sulfate potassium...	13403513	1
Phönix Gotha	Quinolinol sulfate potassium...	140804	1
Dermopharm AG/Noweda	Quinolinol sulfate potassium...	140804	1
Dermapharm	Quinolinol sulfate potassium...	1470804	1
Noweda	Quinolinol sulfate potassium...	140804	2
Bombastus	Quinolinol sulfate potassium...	140804	3
Pharmachen	Quinolinol sulfate potassium...	140804	1
Fagron	Quinolinol sulfate potassium...	140804	2
Euro OTC	Quinolinol sulfate potassium...	140804	2
Caelo	Quinolinol sulfate potassium...	15147704	3
Caelo	Quinolinol sulfate potassium...	15147701	2
Bomb/Gehe	Quinolinol sulfate potassium...	140804	1
Geilenkirchen/Dermopham	Quinolinol sulfate potassium...	140804	1
phönix	Quinolinol sulfate potassium...	140804	1
Mibe/Gehe	Quinolinol sulfate potassium...	140804	1
Caelo	Quinolinol sulfate potassium...	140804	4
Caelo	Quinolinol sulfate potassium...	15147706	3
siehe Protokoll	Quinolinol sulfate potassium...	140804	1
Ebert-Jacobi	Quinolinol sulfate potassium...	16221804	1
Caelo	Quinolinol sulfate potassium...	15147708	4
Caelo	Quinolinol sulfate potassium...	15147714	1
GEHE	Quinolinol sulfate potassium...	15147706	1
Caelo	Quinolinol sulfate potassium...	16221807	1
Caelo	Quinolinol sulfate potassium...	16221804	1
Caelo	Quinolinol sulfate potassium...	16221809	2

- 78 747 spectra from 565 *Apo-Ident* customers from a total of 26 118 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Quinolinol sulfate potassium - sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinolinol sulfate potassium sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	100	0	126 752
Type C	0	104	78	78 736

The substance/substance group *Quinolinol sulfate potassium sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	57.1429 % (> 55.4945 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22606	22626	2.87	78.68
21430	22626	10.85	83.36
22626	22626	0.00	79.01
20983	20983	0.00	70.53

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Resocrinol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20938-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Resocrinol; Resorcinolum

Special notes

When selecting the *Resocrinol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Resocrinol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Resocrinol	12G24-N04	20938	40	1401462
Caelo	Resocrinol	13293108	21471	40	AR-15-FG-006906-01
Fagron	Resocrinol	13I18-B09-291533	21706	30	20130606

Validation samples

A total of 280 317 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 *Resocrinol*. These samples are listed above in the [calibration samples](#) section.
- 74 386 spectra from a total of 1620 batches from further 372 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 [†].

- 115 spectra of 4 reference samples from the substance/substance group *Resocrinol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Resocrinol	13293108	21471 [†]	20
Fagron	Resocrinol	13I18-B09-291533	21706 [†]	15
Caelo	Resocrinol	161533	22632	40
Fagron	Resocrinol	17H03-B11-338899	23921	40

- 126 777 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 123 spectra from 86 *Apo-Ident* customers from 60 batches from the substance/substance group *Resocrinol*.

Supplier	Substance	Batch	Spectra
Caelo	Resocrinol	10218809	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	Resocrinol	11d29-n14	2
Gehe	Resocrinol	11L13-N02	1
Fagron	Resocrinol	11/13-no2	1
Fagron	Resocrinol	11A19-N09	1
Caelo	Resocrinol	10111210	1
Fagron	Resocrinol	2112I-02170	1
Caelo	Resocrinol	5052	1
Caelo	Resocrinol	11309610	4
Fagron	Resocrinol	11L19-N19	2
Fagron	Resocrinol	12G24-N04	10
Fagron	Resocrinol	12G24-N004	1
Caelo	Resocrinol	12G24-N04	2
vdl	Resocrinol	12G24-N04	1
Caelo	Resocrinol	206370-0003	1
Fagron	Resocrinol	12K30-N03	4
Caelo	Resocrinol	19061305	1
Fagron	Resocrinol	12g24-N04	1
Fagron	Resocrinol	11/13-N02	2
Fagron	Resocrinol	1112013A	1
Euro OTC	Resocrinol	11/13-N02	1
Fagron	Resocrinol	13E24-N10	8
Gehe	Resocrinol	13E24-N10	1
Noweda	Resocrinol	13E24-N10	1
Caelo	Resocrinol	13293103	1
Caelo	Resocrinol	12255614	2
Fagron	Resocrinol	13I18-B09	2
Fagron	Resocrinol	13/18-B09-291534	1
Fagron	Resocrinol	13/17071	1
Caelo	Resocrinol	13/18-B19-291534	1
Noweda	Resocrinol	1318b09291533	1
Fagron	Resocrinol	14/16062	1
Fagron	Resocrinol	118b09291534	1
Caelo	Resocrinol	13293110	1
Fagron	Resocrinol	14G10-B06-296296	5
Fagron	Resocrinol	14G10-B06-296297	2
Caelo	Resocrinol	2041512	1
Fagron	Resocrinol	14G10B06	1
Fagron	Resocrinol	13I18-B09-291534	1
Phoenix goettin	Resocrinol	13I18-B09-291534	1
Phoenix WE: 13.07.2015	Resocrinol	14G10-B06-296296	1
Fagron	Resocrinol	13I18-B09-291533	1
Caelo	Resocrinol	15009502	1
Caelo	Resocrinol	13293115	2
Fagron	Resocrinol	14/19050	1
Caelo	Resocrinol	15009507	6
Phönix Gotha	Resocrinol	14G10-B06-296296	1
Fagron	Resocrinol	14J15-B02-307749	5
Fagron	Resocrinol	14J15-B02	1
Fagron	Resocrinol	10B01-N06	2
Fagron	Resocrinol	15K24-B02-317584	2
Fargon	Resocrinol	15K24-B02-317584	1
Caelo	Resocrinol	15K24-B02-317584	1
Caelo	Resocrinol	15009511	2
Fagron	Resocrinol	15/18082	1
Caelo	Resocrinol	15009515	1
Sanacorp	Resocrinol	16D29-B01-323046	1
Fagron	Resocrinol	16D29-B01-323046	1
Fagron	Resocrinol	16D29-B01-329760	3
Fagron	Resocrinol	16d29b01323046	1
Noweda	Resocrinol	14G10-B06-296	1

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Supplier	Substance	Batch	Spectra
Caelo	Resocrinol	18111703	1
Caelo	Resocrinol	16153309	3
Fagron	Resocrinol	16D29-B01-332738	2
Noweda/Fargon	Resocrinol	16029-B01-329760	1
Fagron	Resocrinol	16d29b01332738	1
Fagron	Resocrinol	18B08-B05-347787	2
Caelo	Resocrinol	18015601	1
Caelo	Resocrinol	16153312	1
Caelo	Resocrinol	18216601	1

- 78 806 spectra from 565 *Apo-Ident* customers from a total of 26 078 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Resocrinol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Resocrinol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 386
Type B	0	115	0	126 777
Type C	0	123	0	78 806

The substance/substance group *Resocrinol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 94.5455 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.7826 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 95.1220 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20938	20938	0.00	35.80
21471	21471	0.00	30.88
21706	21471	5.42	26.08

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ribavirin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22346-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ribavirin; Ribavirinum

Special notes

When selecting the *Ribavirin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Ribavirin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ribavirin	1304027-01	22346	30	AR-16-FG-007485-01
Euro OTC	Ribavirin	1308001	22382	30	20130902*
Euro OTC	Ribavirin	1604012	22528	40	20160428*

Validation samples

A total of 280 317 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 *Ribavirin*. These samples are listed above in the [calibration samples](#) section.
- 74 396 spectra from a total of 1620 batches from further 372 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 [†].

- 70 spectra of 3 reference samples from the substance/substance group *Ribavirin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ribavirin	1304027-01	22346 [†]	15
Euro OTC	Ribavirin	1308001	22382 [†]	15
Euro OTC	Ribavirin	1304027-02	23023	40

- 126 822 spectra from a total of 2786 batches from further 781 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 *Ribavirin*.

*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*.

- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ribavirin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ribavirin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 396
Type B	0	70	0	126 822
Type C	0	0	0	78 929

The substance/substance group *Ribavirin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 91.4286 %)
Type C	100.0000 % (> 99.8817 %)	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
22346	22346	0.00	22.37
22382	22382	0.00	26.40
22528	22528	0.00	19.87

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Riboflavin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20409-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Riboflavin; Riboflavinum

Special notes

When selecting the *Riboflavin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Riboflavin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Riboflavin	13D02-N03	20825	40	AR-15-FG-000733-01
AppliChem	Riboflavin	3E003567	20893	40	20130128
Caelo	Riboflavin	12003317	20925	40	1405155
Caelo	Riboflavin	13305203	21389	40	AR-15-FG-005686-01
Fagron	Riboflavin	15G20-B13-310997	21955	40	20150819

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Riboflavin	14322008	22492	40	AR-16-FG-013669-01
Fagron	Riboflavin	16B18-B06-319026	22655	40	AR-16-FG-014466-01
Euro OTC	Riboflavin	1701050	23004	40	20170214*
Fagron	Riboflavin	17G14-B05-337885	23714	40	AR-18-FG-000141-01

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Riboflavin*. These samples are listed above in the [calibration samples](#) section.
- 74136 spectra from a total of 1614 batches from further 372 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 10 reference samples from the substance/substance group *Riboflavin*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Riboflavin	13D02-N03	20914	40
Caelo	Riboflavin	13305203	21389 [†]	20
Fagron	Riboflavin	15G20-B13-310997	21955 [†]	20
Euro OTC	Riboflavin	1701050-01	23091	40
Caelo	Riboflavin	15330708	23579	40
Euro OTC	Riboflavin	1707017	23612	40
Caelo	Riboflavin	172722	23649	40
Euro OTC	Riboflavin	1801018	23880	40
Euro OTC	Riboflavin	1809004	24297	40
Euro OTC	Riboflavin	1810005	24307	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*.

- 126 532 spectra from a total of 2779 batches from further 781 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.

- 17 spectra from 14 *Apo-Ident* customers from 16 batches from the substance/substance group *Riboflavin*.

Supplier	Substance	Batch	Spectra
Euro OTC	Riboflavin	L1305039-01	1
Fagron	Riboflavin	13J29-B04-287534	1
Euro OTC	Riboflavin	L1210048-01	1
Vdl 09.05.14;Preis 7,45	Riboflavin	13305203/15R05	1
Fagron	Riboflavin	13J29-B04-287533	1
Fagron	Riboflavin	167720-0005	1
Fagron	Riboflavin	14B03B07292071	1
Fagron	Riboflavin	14K03-B04-304718	1
Fagron	Riboflavin	15G20-B13-310997	2
Fagron	Riboflavin	15I09-B02-315216	1
Fagron	Riboflavin	16B18b06319026	1
Fagron	Riboflavin	14E01-B10-296718	1
Caelo	Riboflavin	15330708	1
Caelo	Riboflavin	17G14-B05-337885	1
Euro OTC	Riboflavin	1707017-01	1
Anzag/Anzag 11.09.18	Riboflavin	18B22-B01-347142	1

- 78 912 spectra from 565 *Apo-Ident* customers from a total of 26 121 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Riboflavin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Riboflavin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	74 136
Type B	0	360	0	126 532
Type C	0	17	0	78 912

The substance/substance group *Riboflavin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.8817 %)	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
23714	23714	0.00	24.20
20825	20825	0.00	25.80
22492	22492	0.00	26.26
22655	22655	0.00	25.41
23004	23004	0.00	21.50
20893	22492	7.79	24.15
20925	20925	0.00	27.74
21389	21389	0.00	26.24
21955	21389	7.07	25.61

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Riboflavin phosphate sodium**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20948-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Riboflavin phosphate sodium; Natrii lactoflavini phosphoricum

Special notes

When selecting the *Riboflavin phosphate sodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Riboflavin phosphate sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Riboflavin phosp...	13I26-N06	20948	40	1403705
Fagron	Riboflavin phosp...	15J02-B03-313137	22269	40	AR-16-FG-009883-02
Fagron	Riboflavin phosp...	17A03-B01-335897	23713	40	AR-18-FG-000920-01

Validation samples

A total of 280317 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 *Riboflavin phosphate sodium*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 [†].

- 105 spectra of 3 reference samples from the substance/substance group *Riboflavin phosphate sodium*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Riboflavin phosphate sodium	14J31-B07-300519	21707	45
Fagron	Riboflavin phosphate sodium	15J02-B03-313137	22269 [†]	20
Fagron	Riboflavin phosphate sodium	17H03-B13-347175	24113	40

- 126787 spectra from a total of 2786 batches from further 781 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 *Riboflavin phosphate sodium*.
- 78929 spectra from 565 *Apo-Ident* customers from a total of 26137 batches from a further 694 substances. These spectra were 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 *Riboflavin phosphate sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Riboflavin phosphate sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	93	12	126 787
Type C	0	0	0	78 929

The substance/substance group *Riboflavin phosphate sodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	88.5714 % (> 85.7143 %)
Type C	100.0000 % (> 99.8817 %)	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
20948	20948	0.00	13.86
22269	22269	0.00	17.01
23713	23713	0.00	17.52

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Saccharin sodium**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20200-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Saccharin sodium; Saccharinum natricum; Sodium saccharin

Special notes

When selecting the *Saccharin sodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Saccharin sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Saccharin sodium	13I20-B06-291654	23020	40	AR-17-FG-012457-01
Fagron	Saccharin sodium	14F30-B02-296322	23452	40	AR-17-FG-022421-01
Fagron	Saccharin sodium	14F30-B02-296322	23453	40	AR-18-FG-007117-02
Caelo	Saccharin sodium	172110	23643	40	20170831*
Caelo	Saccharin sodium	162210	23857	39	20160811*
Caelo	Saccharin sodium	172592	24409	40	20171206*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 239 spectra of 6 reference samples from the substance/substance group *Saccharin sodium*. These samples are listed above in the [calibration samples](#) section.
- 74 257 spectra from a total of 1618 batches from further 372 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 *Saccharin sodium*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Saccharin sodium	15087704	22769	40
Caelo	Saccharin sodium	182104	24381	40

- 126 812 spectra from a total of 2787 batches from further 781 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 84 *Apo-Ident* customers from 38 batches from the substance/substance group *Saccharin sodium*.

*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
Fargon	Saccharin sodium	12A13-N03	1
Caelo	Saccharin sodium	11172814	1
Caelo	Saccharin sodium	11172805	2
Caelo	Saccharin sodium	90542309	1
Caelo	Saccharin sodium	11025610	1
Caelo	Saccharin sodium	11025605	1
Fagron	Saccharin sodium	12K26-N09	1
Fagron	Saccharin sodium	12A13-N03	1
Caelo	Saccharin sodium	12139803	1
Fagron	Saccharin sodium	SH349/12	1
Caelo	Saccharin sodium	1236207	1
Caelo	Saccharin sodium	12362607	3
Fagron	Saccharin sodium	13D19-N01	1
Caelo	Saccharin sodium	13205414	3
Caesar & Loretz GmbH Hi...	Saccharin sodium	13205418	2
Caelo	Saccharin sodium	14029705	5
sanacorp	Saccharin sodium	13205418	1
Caelo	Saccharin sodium	14029707	3
Sana 03.11.14 EK 3,95	Saccharin sodium	14029707	1
Caelo	Saccharin sodium	14029710	3
Caelo	Saccharin sodium	14213402	2
Caelo	Saccharin sodium	1402970	1
Caelo	Saccharin sodium	13205411	1
Caelo	Saccharin sodium	14213405	5
Caelo	Saccharin sodium	15084101	4
Caesar&loretz,Phoenix	Saccharin sodium	15084101	1
Caelo	Saccharin sodium	15087703	5
Caelo	Saccharin sodium	15087704	9
Caelo	Saccharin sodium		1
Caelo	Saccharin sodium	21092015A	1
Euro OTC	Saccharin sodium	15087704	1
Cael Sanacorp 05.02.2016	Saccharin sodium	15087703	1
Caelo	Saccharin sodium	15087713	14
Jenne	Saccharin sodium	15087707	1
Caelo	Saccharin sodium	14029709	1
Caelo	Saccharin sodium	16221005	7
Caelo	Saccharin sodium	16221010	1
Ichthyol-Gesellschaft	Saccharin sodium	16221009	1
Caelo	Saccharin sodium	17211002	6
Caelo	Saccharin sodium	17211001	2
Caelo	Saccharin sodium	16221009	1
Sanacorp	Saccharin sodium	17211002	1
17270001	Saccharin sodium	17211002	1
Caelo	Saccharin sodium	17329405	1
Cealo	Saccharin sodium	17329405	1
Cealo/ Noweda	Saccharin sodium	17329407	1
Caelo	Saccharin sodium	8121801	1
Kehr	Saccharin sodium	17329407	1
Caelo	Saccharin sodium	17329407	1

- 78 821 spectra from 565 *Apo-Ident* customers from a total of 26 099 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Saccharin sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Saccharin sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	239	0	74 257
Type B	0	80	0	126 812
Type C	0	83	25	78 821

The substance/substance group *Saccharin sodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.4895 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8817 %)	76.8519 % (> 74.0741 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
23020	23020	0.00	86.61
23452	23452	0.00	96.95
23453	23453	0.00	94.52
23643	23643	0.00	78.95
23857	23857	0.00	79.46
24409	24409	0.00	81.62

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Salicylic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20015-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Salicylic acid; Acidum salicylicum

Special notes

When selecting the *Salicylic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Salicylic acid	1110020-01	20696	40	20120125
Caelo	Salicylic acid	13344018	21760	40	20131020
Euro OTC	Salicylic acid	1509007	21906	40	20150929*
Caelo	Salicylic acid	160109	22443	40	20160229*
Fagron	Salicylic acid	16I15-B08-333932	23592	40	20170210

Validation samples

A total of 280317 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 *Salicylic acid*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 [†].

- 420 spectra of 11 reference samples from the substance/substance group *Salicylic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Salicylic acid	13344002	21436	60
Caelo	Salicylic acid	13344018	21760 [†]	20
Euro OTC	Salicylic acid	1509007	21906 [†]	20
Caelo	Salicylic acid	160109	22443 [†]	20
Caelo	Salicylic acid	160500	22448	60
Euro OTC	Salicylic acid	1605023	22685	40
Caelo	Salicylic acid	171333	23277	40
Euro OTC	Salicylic acid	1707009	23556	40
Caelo	Salicylic acid	173015	23827	40
Euro OTC	Salicylic acid	1801042	23968	40
Caelo	Salicylic acid	182300	24236	40

- 126472 spectra from a total of 2778 batches from further 781 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.

- 1427 spectra from 428 *Apo-Ident* customers from 323 batches from the substance/substance group *Salicylic acid*.

Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	11197103	1
Caelo	Salicylic acid	10355916	1
Caelo	Salicylic acid	10291803	1
Caesar&lorenz,Phoenix	Salicylic acid	9220710	1
Caesar&lorenz,Phoenix	Salicylic acid	11197104	1
Gehe	Salicylic acid	11D15-N08	1
Spangropharm	Salicylic acid	11197104	1
Caelo	Salicylic acid	11311902	2
Fagron	Salicylic acid	11K10-N01	2
Caesar & Lorenz GmbH D-...	Salicylic acid	11311904	1
Caelo	Salicylic acid	11311903	1
Fagron	Salicylic acid	12C20-N12	5
Caelo	Salicylic acid	11197117	1
Euro OTC	Salicylic acid	1110020-01	4
Caelo	Salicylic acid	11311910	2
Caelo	Salicylic acid	11311906	2
VDL	Salicylic acid	11197122	1
Caelo	Salicylic acid	11197106	1
Fagron	Salicylic acid	11197121	1
EuRho	Salicylic acid	1206007-01	2
Caelo	Salicylic acid	11197123	4
Fagron	Salicylic acid	3111Q-01045	1
Caelo	Salicylic acid	12036202	3
Jenne	Salicylic acid	12345	1
Caelo	Salicylic acid	9220715	1
Caelo	Salicylic acid	10001612	1
Caelo	Salicylic acid	11311922	9
Phönix	Salicylic acid	11311917	1
Fagron	Salicylic acid	12H10-N08	3
Sanacorp	Salicylic acid	11311922	1
Caelo	Salicylic acid	11311905	1
Caelo	Salicylic acid	20270312-2	1
Caelo	Salicylic acid	20151112-4	1
Phönix	Salicylic acid	12C20-N12	1
Caelo	Salicylic acid	12H10-N08	5
Caelo	Salicylic acid	11197118	1
Caelo	Salicylic acid	1197106	1
Caelo	Salicylic acid		5
Caelo	Salicylic acid	7466	1
Caelo	Salicylic acid	1738980	1
Caelo	Salicylic acid	12036209	4
Euro OTC	Salicylic acid	1206007-01	7
Caelo	Salicylic acid	12036208	1
Caelo	Salicylic acid	12036210	3
Caelo	Salicylic acid	3111J01045	1
Caelo	Salicylic acid	11311917	4
Fagron	Salicylic acid	12H10-N03	6
Caelo	Salicylic acid	12134702	12
Caelo	Salicylic acid	12036211	3
Fagron	Salicylic acid	xxxxxxx	1
Caelo	Salicylic acid	12036315	1
Fagron	Salicylic acid	13B14-N01	16

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Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	12036217	2
Fagron	Salicylic acid	102455-0002	1
Gehe	Salicylic acid	1050313	1
Caelo	Salicylic acid	12036223	7
Caesar & Loretz GmbH, 4...	Salicylic acid	11311917	1
Sanacorp	Salicylic acid	12134707	1
Caelo	Salicylic acid	12134707	6
Caelo	Salicylic acid	12134709	22
Euro OTC	Salicylic acid	115465478596	1
Caelo	Salicylic acid	10355911	2
Sanacorp	Salicylic acid	123036223	1
Caesar&loretz,Anzag	Salicylic acid	12036211	1
Caesar & Loretz GmbH	Salicylic acid	11311922	1
Caelo	Salicylic acid	25041304	1
Alliance Healthcare	Salicylic acid	12036215	2
Caelo	Salicylic acid	4010Q-01045	1
Caelo	Salicylic acid	12036215	2
Caelo	Salicylic acid	11311923	2
Caelo	Salicylic acid	12323402	2
Phoenix	Salicylic acid	12H10-No8	1
Noweda	Salicylic acid	12036215	1
Noweda	Salicylic acid	12036226	1
Eurho/Phoenix	Salicylic acid	13B14-N01	2
Caelo	Salicylic acid	A-100513-1	1
Gehe	Salicylic acid	1206007-01	1
Caelo	Salicylic acid	12036226	7
Caelo	Salicylic acid	12036225	4
Caelo	Salicylic acid	12323401	1
Ichthyol	Salicylic acid	11311922	2
Alliance Healthcare	Salicylic acid	12036216	1
Caelo	Salicylic acid	12036216	5
Caelo	Salicylic acid	12134711	8
Euro OTC	Salicylic acid	1303020-01	18
Phönix	Salicylic acid	12323401	1
Fagron	Salicylic acid	12C20-N04	1
Bombastus	Salicylic acid	12036223	1
Caelo	Salicylic acid	12374205	7
Caelo	Salicylic acid	1234709	1
Caelo	Salicylic acid	13B14-No1	1
Fagron	Salicylic acid	13H01-N01	6
Caelo	Salicylic acid	12134714	16
Caelo	Salicylic acid	9091301	1
Bombastus	Salicylic acid	12323403	1
Caelo	Salicylic acid	123134712	1
Euro OTC	Salicylic acid	1110020	1
Caelo	Salicylic acid	12134712	4
Gehe	Salicylic acid	13B14-N01	1
Fagron	Salicylic acid	13H01-N08	2
Sanacorp	Salicylic acid	12374205	1
Caelo	Salicylic acid	12374204	1
Europ Ots Pharma	Salicylic acid	12374205	1
carlo	Salicylic acid	12134714	2
Caesar&Loretz GmbH/Anzag	Salicylic acid	12374204	1
Caelo	Salicylic acid	9112013A	1
Caelo	Salicylic acid	12374210	3
Caelo	Salicylic acid	20111306	1
Sanacorp	Salicylic acid	12134712	1
Phönix Gotha	Salicylic acid	12374207	1
Caelo	Salicylic acid	12134710	1
Caelo	Salicylic acid	12134717	9

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Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	12374207-3454311172	1
Caelo	Salicylic acid	12323403	3
Caelo	Salicylic acid	1913Q-01045	1
Fagron	Salicylic acid	13H01N01	1
Caelo	Salicylic acid	10355912	1
Caelo	Salicylic acid	12374207	5
Caelo	Salicylic acid	13H01-N01	1
Caelo	Salicylic acid	12134713	1
Caelo	Salicylic acid	12134715	7
Fagron	Salicylic acid	13H01-N04	13
Fagron	Salicylic acid	RAS1135300	1
Phönix	Salicylic acid	1303020-01	3
Caelo	Salicylic acid	1234	1
Caelo	Salicylic acid	13H01-N04	2
Caelo	Salicylic acid	12374211	17
Sanacorp	Salicylic acid	12374210	1
Sanacorp	Salicylic acid	12134715	1
Caelo	Salicylic acid	12134719	3
Caelo	Salicylic acid	13032014A	1
Sanacorp	Salicylic acid	1303020-01	1
Caelo	Salicylic acid	12134720	8
Phönix	Salicylic acid	12374211	1
Anzag	Salicylic acid	1303020-01	2
Caelo	Salicylic acid	12374213	11
Fagron	Salicylic acid	13H01N04	4
Phönix	Salicylic acid	12374210	1
Caelo	Salicylic acid	1274210	1
Caelo	Salicylic acid	3601413011-12374211	1
Caesar & Loretz GmbH Hi...	Salicylic acid	12134714	1
Gutenberg-Apotheke	Salicylic acid	12374208	1
Caelo	Salicylic acid	12374208	2
Caelo	Salicylic acid	1714Q1045	1
Caelo	Salicylic acid	12374212	2
Fagron	Salicylic acid	13K08-B31-290852	5
Caelo	Salicylic acid	12134721	2
Euro OTC	Salicylic acid	130302001	1
Caelo	Salicylic acid	13344002	19
Gehe	Salicylic acid	13H01-N04	1
Klenk	Salicylic acid	12134722	1
Fagron	Salicylic acid	14B05-B30-290854	4
Caelo	Salicylic acid	14076201	1
Caelo	Salicylic acid	1334403	1
Sanacorp	Salicylic acid	68/AKD2	1
Caelo	Salicylic acid	7071403	1
Caelo	Salicylic acid	13344003	9
Euro OTC	Salicylic acid	1303020-02	4
Caelo	Salicylic acid	1303020-01	2
Caelo	Salicylic acid	14076203	6
AHD 22.07.14	Salicylic acid	134002	1
Fagron	Salicylic acid	13K08-B31-290853	4
Caelo	Salicylic acid	16072014A	1
Caelo	Salicylic acid	12134722	4
Caelo	Salicylic acid	133454002	1
Phönix	Salicylic acid	13K08-B31-290853	1
Caelo	Salicylic acid	14076206	6
Caelo	Salicylic acid	14076207	10
Euro OTC	Salicylic acid		1
Farmalabor / Farmalabor	Salicylic acid	P1404195-002	1
Caelo	Salicylic acid	14076204	10
Phönix Gotha	Salicylic acid	14076201	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Salicylic acid	102455	1
AHD	Salicylic acid	13344002	1
Phoenix	Salicylic acid	14076201	1
Caelo	Salicylic acid	13344014	6
Caelo	Salicylic acid	10355907	1
Caelo	Salicylic acid	10112014B	1
Caelo	Salicylic acid	14076211	1
Fagron	Salicylic acid	290852	1
Fagron	Salicylic acid	14E26-B04-294623	6
Fagron	Salicylic acid	14B05-B30	2
xxx	Salicylic acid	4311A-01045	1
Fagron	Salicylic acid	14E26-B04-294624	6
Holdermann	Salicylic acid	14E26-B04294624	1
Caelo	Salicylic acid	18121412	1
Caelo	Salicylic acid	14300801	5
Caelo	Salicylic acid	13344013	10
Caelo	Salicylic acid	14076202	6
Euro OTC	Salicylic acid	1406027-01	8
Fagron	Salicylic acid	14E26-B04	5
Alliance 19.12.12	Salicylic acid	11311906	1
Sanacorp	Salicylic acid	13344014	1
Sanacorp 28.01.15 EK 12...	Salicylic acid	14076204	1
Caesar&Loretz GmbH/Anzag	Salicylic acid	14076203	2
Caelo	Salicylic acid	140602701	1
Caelo	Salicylic acid	14300802	6
Fagron	Salicylic acid	14e26-B04-294623	1
Caelo	Salicylic acid	13344018	18
Caelo	Salicylic acid	13344020	15
Caelo	Salicylic acid	1430802	1
Fagron	Salicylic acid	14E26B04294623	1
Fagron	Salicylic acid	11L19-N21	1
Caesar & Loretz GmbH	Salicylic acid	13344003	1
Caelo	Salicylic acid	14300806	1
Noweda	Salicylic acid	1406027-01	1
Caelo	Salicylic acid	14300805	10
Caesar&loretz,Phoenix	Salicylic acid	14076212	1
Fagron	Salicylic acid	14E26B04	2
Caelo	Salicylic acid	15084401	3
Caelo	Salicylic acid	14076212	1
14076202	Salicylic acid		1
Caelo	Salicylic acid	14300804	6
Fagron	Salicylic acid	14E26-B04294623	1
Euro OTC	Salicylic acid	1406027-02	10
Fagron	Salicylic acid	14e26-b04-294623	1
Caelo	Salicylic acid	1406027-02	2
Euro OTC	Salicylic acid	140602702	1
Fagron	Salicylic acid	14E26-B04-294622	1
Caesar&Loretz Anzag	Salicylic acid	14300804	2
Phönix	Salicylic acid	68/AKD4	1
Fagron	Salicylic acid	14E26-B04-296424	1
Caelo	Salicylic acid	14300809	11
Euro OTC	Salicylic acid	1406027-02Mg1kg	1
Phoenix goettingen	Salicylic acid	14300808	1
Euro OTC	Salicylic acid	14E26-B04-294622	1
Phönix Gotha	Salicylic acid	14300801	1
Fagron	Salicylic acid	14L02-B02	3
Euro OTC	Salicylic acid	14076202	1
Fagron	Salicylic acid	14B05B30	1
Fagron	Salicylic acid	13344013	1
Caelo	Salicylic acid	23071510	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Salicylic acid	14300809	1
Caelo	Salicylic acid	15084403	7
Caelo	Salicylic acid	15084404	3
Caelo	Salicylic acid	15217301	6
Sanacorp	Salicylic acid	15084404	1
Novacyl, FR	Salicylic acid	15084403	2
Caelo	Salicylic acid	14300808	1
Caelo	Salicylic acid	14336907	21
Caesar&Loretz GmbH/Sana...	Salicylic acid	15217301	1
Caelo	Salicylic acid	15217302	14
ACM	Salicylic acid	KNC0461J15	1
Caelo	Salicylic acid	14336906	3
Fagron	Salicylic acid	14L02-B02-303557	10
Caelo	Salicylic acid	15217303	9
Anzag/Henry Lamotte	Salicylic acid	1334018	1
EuRho	Salicylic acid	1406027-01	2
Euro OTC	Salicylic acid	1408027	1
Caelo	Salicylic acid	14336905	12
Caelo	Salicylic acid	15217304	4
Gehe	Salicylic acid	14L02-B02-303558	1
Caelo	Salicylic acid	14336904	1
Caelo	Salicylic acid	15217305	6
Noweda	Salicylic acid	140602702	1
Fagron	Salicylic acid	14L02-B02-303558	9
Euro OTC	Salicylic acid	1509007-01	25
Caelo	Salicylic acid	15217308	8
Caelo	Salicylic acid	152117304	1
Noweda	Salicylic acid	14336907	2
caesar	Salicylic acid	15217301	1
Fargon	Salicylic acid	14L02-B02	1
Caelo	Salicylic acid	15211806	2
Caelo	Salicylic acid	15211809	10
Caelo	Salicylic acid	14336908	1
Fagron	Salicylic acid	2201115	1
Caelo	Salicylic acid	1509007-01	1
Caelo	Salicylic acid	15211810	6
Caelo	Salicylic acid	14336911	17
Fagron	Salicylic acid	14L02B02303557	1
EurRho/ Anzag	Salicylic acid	1509007-01	1
Caelo	Salicylic acid	15211808	8
Euro OTC	Salicylic acid	15217301	1
Ichthyol/Noweda	Salicylic acid	13344003	1
Caelo	Salicylic acid	151224/1	1
Caelo	Salicylic acid	14336911	1
Caelo	Salicylic acid	14336912	7
EuRho	Salicylic acid	1406027-02	1
Caelo	Salicylic acid	16010903	8
Euro	Salicylic acid	1509007-02	1
Phoenix	Salicylic acid	15211808	2
Caelo	Salicylic acid	16010907	5
Caelo	Salicylic acid	15211807	2
Euro OTC	Salicylic acid	1509007-02	9
Fagron	Salicylic acid	14L02B02303558	1
Caelo	Salicylic acid	1310516	1
Fagron	Salicylic acid	1140616	1
Caelo	Salicylic acid	14336919	17
Caelo	Salicylic acid	16010905	9
EuRho	Salicylic acid	1303020-01	1
Caelo	Salicylic acid	14336921	1
Fagaron	Salicylic acid	14Lo2-B02-303558	1

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Supplier	Substance	Batch	Spectra
Phönix	Salicylic acid	1509007-02	1
Caelo	Salicylic acid	16050003	2
Caesar&Loretz/AHD	Salicylic acid	15211808	1
Caelo	Salicylic acid	14336920	18
Euro OTC	Salicylic acid	1509007/02	1
Caelo	Salicylic acid	15081601	1
Caolo- Noweda	Salicylic acid	14300809	2
Ebert 24.08.16	Salicylic acid	16010903	1
EuRho 001	Salicylic acid	1509007-02	1
Fagron	Salicylic acid	16A18-B04-322905	1
Krieger	Salicylic acid	16050012	1
Caelo	Salicylic acid	16010906	11
Caelo	Salicylic acid	16010901	3
Caelo	Salicylic acid	160405AS	1
Fagron	Salicylic acid	16A18-B04	1
Caelo	Salicylic acid	16050004	11
Caelo	Salicylic acid	160500004	3
Euro OTC	Salicylic acid	1605023-01	13
Caelo	Salicylic acid	16010904	8
Fagron	Salicylic acid	16A18-B04322904	1
Caelo	Salicylic acid	16010908	1
Caelo	Salicylic acid	16E02-B09-325355	1
Phönix	Salicylic acid	16a18-b04-322905	1
Caelo	Salicylic acid	Validierungsmessung	1
Caelo	Salicylic acid	16050005	8
EuRho	Salicylic acid		1
Celo/ Sanacorp	Salicylic acid	16010908	1
Alliance Healthcare	Salicylic acid	15211808	1
Caelo	Salicylic acid	16050011	9
Gehe / Spinnrad	Salicylic acid	16050005	1
Caelo	Salicylic acid	1045	1
Euro OTC	Salicylic acid	16E02-B09-325356	1
Fagron	Salicylic acid	16A18-B04-322904	2
Caelo	Salicylic acid	15211803	1
Caelo	Salicylic acid	16010913	12
Caelo	Salicylic acid	16010912	2
Sana 04.02.17 Ek:13,83	Salicylic acid	16010910	1
Caelo	Salicylic acid	16010917	13
Caelo	Salicylic acid	16050012	8
Caelo	Salicylic acid	16010910	9
Sanacorp	Salicylic acid	16010910	1
Euro OTC	Salicylic acid	160502301	2
Caelo	Salicylic acid	RAS1135100	1
Bombastus	Salicylic acid	1605023-01	1
Phönix	Salicylic acid	16050005	1
Krieger	Salicylic acid	13032017-MW-A	1
Caelo	Salicylic acid	3816Q-01045	1
Fagron	Salicylic acid		1
Caelo	Salicylic acid	16010916	1
Noweda/ Infecto Pharm	Salicylic acid	16/15-08-330773	1
Euro OTC	Salicylic acid	1605023/02	1
Caelo	Salicylic acid	1600917	1
Fagron	Salicylic acid	16/15-B08-330773	3
Caelo	Salicylic acid	1605023-01	1
Fagron	Salicylic acid	16I15-B08-327353	1
Caelo	Salicylic acid	16010911	4
Fagron	Salicylic acid	16I15-B08	1
Caelo	Salicylic acid	16050013	11
Gehe	Salicylic acid	165023-02	1
Euro OTC	Salicylic acid	1605023-02	9

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Supplier	Substance	Batch	Spectra
Gehe	Salicylic acid	16010910	1
Caelo	Salicylic acid	16010918	7
Fagron	Salicylic acid	16I15-B08-330773	1
Caelo	Salicylic acid	16I15-B08	1
Noweda	Salicylic acid	16050011	1
Caelo	Salicylic acid	16010923	4
Caelo	Salicylic acid	170509AS/16050012	1
Fagron	Salicylic acid	15211809	1
Fagron	Salicylic acid	16/15-B08-332098	2
Caelo	Salicylic acid	16312001	15
Caelo	Salicylic acid	16010972	1
Caelo	Salicylic acid	16050014	13
GEHE	Salicylic acid	1605023-02	2
Caelo	Salicylic acid	1601916	1
Caelo	Salicylic acid	8170717	1
gehe	Salicylic acid	16I15-B08-331442	1
Caelo	Salicylic acid	16010922	6
Caelo	Salicylic acid	160109123	1
Caesar&Loretz GmbH,15.0...	Salicylic acid	16312001	1
Caesar & Loretz GmbH	Salicylic acid	16312001	1
Anzag	Salicylic acid	16050014	1
Noweda	Salicylic acid	16050013	1
Fagron	Salicylic acid	16I15-B08-333932	1
GEHE	Salicylic acid	1605023-01	1
Caelo	Salicylic acid	16312003	5
Bombastus	Salicylic acid	16050017	1
Cealo	Salicylic acid	15211806	1
Caelo	Salicylic acid	16312005	10
Caelo	Salicylic acid	16050017	10
apo ident	Salicylic acid	1605023-01	1
Caelo	Salicylic acid	13101707	1
Caelo	Salicylic acid	207102017/16050017	1
Euro OTC	Salicylic acid	1707009-01	11
Caelo	Salicylic acid	17133303	9
Caelo	Salicylic acid	17133301	4
Caelo	Salicylic acid	163120	1
Caelo	Salicylic acid	16312010	11
Caelo	Salicylic acid	16312009	7
Fagron	Salicylic acid	17C21-B09	2
GEHE	Salicylic acid	1707009-01	1
Kehr	Salicylic acid	16312001	2
Fagron	Salicylic acid	17C21-B09-337173	2
Caelo	Salicylic acid	1707009-01	1
Caelo	Salicylic acid	17301505	9
Phoenix/Cealo	Salicylic acid	1733303	1
Phoenix/Cealo	Salicylic acid	3414M-01045	1
Caelo	Salicylic acid	14E26-B04-294622	1
Caelo	Salicylic acid	17301504	2
Fagron	Salicylic acid	17C21B09	1
Caelo	Salicylic acid	1713301	1
Fagron	Salicylic acid	16I15-B08-332098	1
Euro OTC	Salicylic acid	1707009-02	2
Caelo	Salicylic acid	17301503	7
Caelo	Salicylic acid	17133307	17
Caelo	Salicylic acid	16312008	1
GEHE	Salicylic acid	1707009-02	1
Caelo	Salicylic acid	17301502	5
Caelo	Salicylic acid	17301506	8
Caelo	Salicylic acid	17051803	1
Fiebig/Maros	Salicylic acid	1707009-02	1

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Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	17123301	1
Kehr	Salicylic acid	16312012	1
Sanacorp	Salicylic acid	17C21-B09-339446	1
Caelo	Salicylic acid	170301506	1
Delta	Salicylic acid	17133303	1
Caelo	Salicylic acid	18050002	5
Caelo	Salicylic acid	170700902	1
Euro OTC	Salicylic acid	1801042-01	9
Fagron	Salicylic acid	17C21-B09-337860	1
Fiebig	Salicylic acid	17301506	1
euro AHD	Salicylic acid	1707009-025709	1
Noweda/Fargon	Salicylic acid	14L02-B02-303556	1
Caelo	Salicylic acid	18050006	5
Anzag/Anzag 11.09.18	Salicylic acid	18F05-B02-350586	1
Caelo	Salicylic acid	18050007	1
Caelo	Salicylic acid	17301507	5
Euro OTC	Salicylic acid	17301509	1
Sanacorp	Salicylic acid	17301509	1
Sanacorp	Salicylic acid	18050006	1
Caelo	Salicylic acid	1801042-01	1
Caelo	Salicylic acid	16050006	1
Fagron	Salicylic acid	18F05-B02-350586	2
Fagron	Salicylic acid	18E24-B03-354311	1
Caelo	Salicylic acid	17301509	2
Kehr	Salicylic acid	17301509	1
Caelo	Salicylic acid	18050009	2
Caelo	Salicylic acid	RAS1703500	1

- 77 502 spectra from 565 *Apo-Ident* customers from a total of 25 819 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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* can clearly be 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* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	420	0	126 472
Type C	0	1397	30	77 502

The substance/substance group *Salicylic 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 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.5714 %)
Type C	100.0000 % (> 99.8817 %)	97.8977 % (> 97.6875 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20696	21906	3.80	80.38
21760	21906	1.60	83.31
21906	21906	0.00	83.80
22443	22443	0.00	77.08
23592	21906	2.13	81.53

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Selenium yeast**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20906-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Selenium yeast

Special notes

When selecting the *Selenium yeast* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Selenium yeast*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Selenium yeast	L1204012-01	20906	40	1403461
Caelo	Selenium yeast	13347911	21377	40	1509355
Caelo	Selenium yeast	17002202	23120	40	1707512
Caelo	Selenium yeast	173332	24038	40	20180207*

Validation samples

A total of 280 317 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 *Selenium yeast*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Selenium yeast*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Selenium yeast	L1401013-01	21102	40
Caelo	Selenium yeast	17002208	23446	40

- 126 812 spectra from a total of 2787 batches from further 781 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 *Selenium yeast*.

*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
Caesar & Loretz GmbH, 4...	Selenium yeast	11318111	1
Caelo	Selenium yeast	13347906	1
Caelo	Selenium yeast	15276208	1
Caelo	Selenium yeast	13347911	1

- 78 925 spectra from 565 *Apo-Ident* customers from a total of 26 133 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Selenium yeast* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Selenium yeast* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	80	0	126 714
Type C	0	3	1	78 925

The substance/substance group *Selenium yeast* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8820 %)	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
23120	23120	0.00	24.32

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24038	24038	0.00	24.28
20906	20906	0.00	31.81
21377	21377	0.00	30.19

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sildenafil citrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20852-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sildenafil citrate; Sildenafil citras

Special notes

When selecting the *Sildenafil citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Sildenafil citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sildenafil citrate	13F24-N03	20852	40	1402052
Fagron	Sildenafil citrate	13J15-N01	20927	80	20131030
Euro OTC	Sildenafil citrate	1311010-01	21621	40	20131209
Caelo	Sildenafil citrate	160498	22446	40	20160307*
Caelo	Sildenafil citrate	170715	23336	40	20170529*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Sildenafil citrate*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1618 batches from further 372 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 *Sildenafil citrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sildenafil citrate	1311010-01	21621 [†]	20
Caelo	Sildenafil citrate	160498	22446 [†]	20
Euro OTC	Sildenafil citrate	1311010-04	23178	40
Caelo	Sildenafil citrate	170715	23345	40
Euro OTC	Sildenafil citrate	1807037	24192	40

- 126 732 spectra from a total of 2784 batches from further 781 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*.

- 154 spectra from 44 *Apo-Ident* customers from 69 batches from the substance/substance group *Sildenafil citrate*.

Supplier	Substance	Batch	Spectra
Fagron	Sildenafil citrate	13J15-N01	2
Euro OTC	Sildenafil citrate	1311010-01	3
Gehe	Sildenafil citrate	13F24-N03	1
Euro OTC	Sildenafil citrate	14051402	1
Caelo	Sildenafil citrate	14074703	2
Euro OTC	Sildenafil citrate	17061405	1
Phönix/Polpharma	Sildenafil citrate	1311010-01	1
Caelo	Sildenafil citrate	14074707	2
Polpharma/Phoenix	Sildenafil citrate	131101001	1
Gutenberg-Apotheke	Sildenafil citrate	1311010-01	1
Caelo	Sildenafil citrate	14074709	1
Caelo	Sildenafil citrate	2101403	1
Euro OTC	Sildenafil citrate	13110-01	1
Caelo	Sildenafil citrate	1407474	1
Caelo	Sildenafil citrate	14074714	5
Caelo	Sildenafil citrate	14074715	5
Caelo	Sildenafil citrate	14074716	1
Sanacorp	Sildenafil citrate	14H11-B01-297519	2
Euro OTC	Sildenafil citrate	1311010-03	5
Euro OTC	Sildenafil citrate	131101003	1
Fagron	Sildenafil citrate	14H11-B01-303183	1
Euro OTC	Sildenafil citrate	17081504	1
Caelo	Sildenafil citrate	15097301	1
Caelo	Sildenafil citrate	15097306	1
Euro OTC	Sildenafil citrate	15097301	1
Caelo	Sildenafil citrate	15097303	1
Caelo	Sildenafil citrate	15097307	2
Caelo	Sildenafil citrate	15F11-B02-314725	1
Caelo	Sildenafil citrate	15097312	2
Caelo	Sildenafil citrate	15097315	1
Alliance	Sildenafil citrate	1311010-03	1
Caelo	Sildenafil citrate	15F11-B02-309081	1
Phoenix	Sildenafil citrate	1311010-04	2
Euro OTC	Sildenafil citrate	1311010-04	2
Caelo	Sildenafil citrate	16049802	10
Fagron	Sildenafil citrate	15F11-B02-320186	1
Euro OTC	Sildenafil citrate	131101004	1
Fagron	Sildenafil citrate	15F11-B02-314725	1
Caelo	Sildenafil citrate	16049810	1
Gehe	Sildenafil citrate	16049805	1
Fagron	Sildenafil citrate	15f11-b02-320186	1
Caelo	Sildenafil citrate	16049808	3
Caelo	Sildenafil citrate	16049805	1
	Sildenafil citrate	1311010-04	2
Caelo	Sildenafil citrate	16049814	9
Sanacorp	Sildenafil citrate	16049811	2
Caelo	Sildenafil citrate	16049812	1
Sanacorp WE 21.04.17 -2...	Sildenafil citrate	16049808	1
Caelo	Sildenafil citrate	16049821	8
Caelo	Sildenafil citrate	16049819	1
Fagron	Sildenafil citrate	16F30-B02-324715	1
Caelo	Sildenafil citrate	101051528	1
Caelo	Sildenafil citrate	16049820	4
Euro OTC	Sildenafil citrate	10061706	1
Fagron	Sildenafil citrate	16F30-B02-324715	1
Fagron	Sildenafil citrate	16A18-B08	2
Caelo	Sildenafil citrate	16049801	1

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Supplier	Substance	Batch	Spectra
Fagron	Sildenafil citrate	16049817	1
Euro OTC	Sildenafil citrate	1311010-05	3
Euro OTC	Sildenafil citrate	1311010-06	7
Caelo	Sildenafil citrate	16049823	1
Fagron	Sildenafil citrate	16F30-B02-331450	3
Alliance	Sildenafil citrate		1
Caelo	Sildenafil citrate	16049826	1
Fagron	Sildenafil citrate	16049812	1
Fagron	Sildenafil citrate	16049819	2
Fagron	Sildenafil citrate	16F30-B02	1
Caelo	Sildenafil citrate	17071502	1
Caelo	Sildenafil citrate	16049824	1
Fagron	Sildenafil citrate	16F30-B02-334977	1
Caelo	Sildenafil citrate	17071504	6
Fagron	Sildenafil citrate	17071505	1
Fagron	Sildenafil citrate	16F30-B02-331449	1
Fagron	Sildenafil citrate	17H31-B02-342459	3
GEHE	Sildenafil citrate	17344003	1
Euro OTC	Sildenafil citrate	103031328	1
Euro OTC	Sildenafil citrate	27021802	1
Euro OTC	Sildenafil citrate	1311010	1
Euro OTC	Sildenafil citrate	15081830	1
Caelo	Sildenafil citrate	17344003	2
Euro OTC	Sildenafil citrate	19011907	1

- 78 775 spectra from 565 *Apo-Ident* customers from a total of 26 068 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sildenafil citrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sildenafil citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	160	0	126 732
Type C	0	152	2	78 775

The substance/substance group *Sildenafil citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	98.7013 % (> 96.7532 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20852	20852	0.00	67.67
20927	20852	2.89	66.25
21621	20852	7.56	64.90
23336	23336	0.00	65.61
22446	22446	0.00	61.24

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Sodium acetate trihydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20984-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium acetate trihydrate; Natrii acetat trihydricum

Special notes

When selecting the *Sodium acetate trihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	European Pharmacopoeia 9th Edition, Basic Version 2017 [3]
Komm2.2.40	Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident [4]
AA004	Erstellung und Validierung eines IdentModul-Updates
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 acetate trihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium acetate t...	12316506	20984	40	1402111
Caelo	Sodium acetate t...	13411404	21441	40	20140113
Euro OTC	Sodium acetate t...	1507020	21861	40	20150723*
Caelo	Sodium acetate t...	172003	23812	40	20171107*

Validation samples

A total of 280 317 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 acetate trihydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Sodium acetate trihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium acetate trihydrate	13411404	21441 [†]	20
Euro OTC	Sodium acetate trihydrate	1507020	21861 [†]	20
Caelo	Sodium acetate trihydrate	163007	22760	40
Euro OTC	Sodium acetate trihydrate	1608032	22802	40
Euro OTC	Sodium acetate trihydrate	1706008	23547	40
Caelo	Sodium acetate trihydrate	183152	24370	40

- 126 692 spectra from a total of 2783 batches from further 781 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*.

- 40 spectra from 27 *Apo-Ident* customers from 20 batches from the substance/substance group *Sodium acetate trihydrate*.

Supplier	Substance	Batch	Spectra
Caelo	Sodium acetate trihydrate	12027202	1
Caelo	Sodium acetate trihydrate	12027217	1
Caelo	Sodium acetate trihydrate	12027228	1
Caelo	Sodium acetate trihydrate	10353017	1
Caelo	Sodium acetate trihydrate	13295606	1
Phönix Gotha	Sodium acetate trihydrate	12316506	1
Sanacorp	Sodium acetate trihydrate	13295601	1
Caelo	Sodium acetate trihydrate	13295601	1
Caelo	Sodium acetate trihydrate	12316501	1
Caelo	Sodium acetate trihydrate	13411418	2
Caelo	Sodium acetate trihydrate	15118701	3
Caelo	Sodium acetate trihydrate	15145204	5
Caelo	Sodium acetate trihydrate	151452009	1
Caelo	Sodium acetate trihydrate	15145205	1
Caelo	Sodium acetate trihydrate	15145209	5
Ebert KKH 13.10.16	Sodium acetate trihydrate	15145204	1
Caelo	Sodium acetate trihydrate	15145218	1
Ebert KKH 13.10.16	Sodium acetate trihydrate	15145209	1
Caelo	Sodium acetate trihydrate	16300706	2
Caelo	Sodium acetate trihydrate	16300712	1
Caelo	Sodium acetate trihydrate	16300711	3
Euro OTC	Sodium acetate trihydrate	1005020V-01	1
Caesar & Lorenz GmbH	Sodium acetate trihydrate	16300706	1
Caelo	Sodium acetate trihydrate	18006801	3

- 78 889 spectra from 565 *Apo-Ident* customers from a total of 26 117 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 acetate trihydrate* can clearly be 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 acetate trihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	200	0	126 692
Type C	0	38	2	78 889

The substance/substance group *Sodium acetate trihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8817 %)	95.0000 % (> 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
21861	21861	0.00	29.93
20984	20984	0.00	31.32
21441	20984	2.57	31.73
23812	23812	0.00	31.62

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sodium ascorbate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20520-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sodium ascorbate; Natrii ascorbas

Special notes

When selecting the *Sodium ascorbate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 ascorbate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Sodium ascorbate	1406018-01	21583	40	1411165
Euro OTC	Sodium ascorbate	1507030	21853	40	20150811*
Euro OTC	Sodium ascorbate	1506018	21865	40	20150706*
Euro OTC	Sodium ascorbate	1510017	21946	40	20151102*
Euro OTC	Sodium ascorbate	1601007	22304	40	20160120*
Caelo	Sodium ascorbate	15429905	22899	40	20160118

Validation samples

A total of 280 317 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 *Sodium ascorbate*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 [†].

- 720 spectra of 20 reference samples from the substance/substance group *Sodium ascorbate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sodium ascorbate	1406018-01	21583 [†]	20
Euro OTC	Sodium ascorbate	1406018-01	21789	60
Euro OTC	Sodium ascorbate	1507030	21853 [†]	20
Euro OTC	Sodium ascorbate	1506018	21865 [†]	20
Euro OTC	Sodium ascorbate	1510017	21946 [†]	20
Euro OTC	Sodium ascorbate	1601007	22304 [†]	20
Euro OTC	Sodium ascorbate	1604001	22524	40
Euro OTC	Sodium ascorbate	1607044	22690	40
Caelo	Sodium ascorbate	162857	22761	40
Euro OTC	Sodium ascorbate	1611015	22864	40
Euro OTC	Sodium ascorbate	1701054	23134	40
Euro OTC	Sodium ascorbate	1703012	23152	40
Euro OTC	Sodium ascorbate	1705013	23430	40
Euro OTC	Sodium ascorbate	1705014	23432	40
Caelo	Sodium ascorbate	172235	23809	40
Caelo	Sodium ascorbate	180326	24029	40
Euro OTC	Sodium ascorbate	1803005	24069	40
Euro OTC	Sodium ascorbate	1807043	24149	40
Euro OTC	Sodium ascorbate	1811002	24337	40
Caelo	Sodium ascorbate	182620	24386	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*.

- 126 172 spectra from a total of 2770 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 20 spectra from 6 *Apo-Ident* customers from 20 batches from the substance/substance group *Sodium ascorbate*.

Supplier	Substance	Batch	Spectra
Euro OTC	Sodium ascorbate	1210026-01	1
Euro OTC	Sodium ascorbate	28081304	1
Euro OTC	Sodium ascorbate	16091301	1
Euro OTC	Sodium ascorbate	20091303	1
Caelo	Sodium ascorbate	27091302	1
Fagron	Sodium ascorbate	12L27-N03	1
Euro OTC	Sodium ascorbate	11121301	1
Fagron	Sodium ascorbate	13C15-N01	1
Euro OTC	Sodium ascorbate	7011405	1
Euro OTC	Sodium ascorbate	L1308005-01	1
Euro OTC	Sodium ascorbate	4021401	1
Euro OTC	Sodium ascorbate	13031402	1
Euro OTC	Sodium ascorbate	13051406	1
Euro OTC	Sodium ascorbate	12061407	1
Euro OTC	Sodium ascorbate	11081401	1
Caelo	Sodium ascorbate	15180505	1
Caelo	Sodium ascorbate	14079404	1
Caelo	Sodium ascorbate	1604001-01	1
Euro OTC	Sodium ascorbate	170105401	1
Caelo	Sodium ascorbate	16285710	1

- 78 909 spectra from 565 *Apo-Ident* customers from a total of 26 117 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 ascorbate* can clearly be 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 ascorbate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	717	3	126 172
Type C	0	20	0	78 909

The substance/substance group *Sodium ascorbate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	99.5833 % (> 99.1667 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 70.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21583	21583	0.00	86.95
21853	21853	0.00	85.22
21865	21865	0.00	83.50
21946	21946	0.00	85.45
22304	22304	0.00	82.11
22899	22304	1.71	82.30

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Sodium benzoate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20479-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium benzoate; Natrii benzoas

Special notes

When selecting the *Sodium benzoate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 benzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium benzoate	11267016	20752	40	20110923
Caelo	Sodium benzoate	13178619	21607	40	20130624
Euro OTC	Sodium benzoate	1409040-01	21713	40	20141021
Euro OTC	Sodium benzoate	1506019	21825	40	20150623*
Euro OTC	Sodium benzoate	1510044	22236	40	20151109*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Sodium benzoate	1602020	22363	40	20160225*
Euro OTC	Sodium benzoate	1610037	22867	40	20161202*
Euro OTC	Sodium benzoate	1701045	22997	40	20170207*
Euro OTC	Sodium benzoate	1711019	23900	40	20171205*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Sodium benzoate*. These samples are listed above in the [calibration samples](#) section.
- 74136 spectra from a total of 1614 batches from further 372 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 13 reference samples from the substance/substance group *Sodium benzoate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium benzoate	13178619	21607 [†]	20
Euro OTC	Sodium benzoate	1409040-01	21713 [†]	20
Euro OTC	Sodium benzoate	1506019	21825 [†]	20
Euro OTC	Sodium benzoate	1510044	22236 [†]	20
Euro OTC	Sodium benzoate	1602020	22363 [†]	20
Caelo	Sodium benzoate	161371	22474	60
Euro OTC	Sodium benzoate	1607005	22670	40
Fagron	Sodium benzoate	15B16-B07-308570	22895	40
Caelo	Sodium benzoate	170558	23283	40
Euro OTC	Sodium benzoate	1707024	23613	40
Caelo	Sodium benzoate	173530	23784	40
Euro OTC	Sodium benzoate	1803034	24068	40
Euro OTC	Sodium benzoate	1809005	24301	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*.

- 126 452 spectra from a total of 2776 batches from further 781 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.

- 241 spectra from 160 *Apo-Ident* customers from 103 batches from the substance/substance group *Sodium benzoate*.

Supplier	Substance	Batch	Spectra
Fagron	Sodium benzoate	12D02-N06	1
Fagron	Sodium benzoate	test	1
Euro OTC	Sodium benzoate	1112006-01	1
Caelo	Sodium benzoate	1209018-0	1
Euro OTC	Sodium benzoate	1209018-18	1
Euro OTC	Sodium benzoate	1209018-01	4
Fagron	Sodium benzoate	12G04-N04	1
Fagron	Sodium benzoate	12C05-N04	1
Euro OTC	Sodium benzoate	1007019-01	1
Caelo	Sodium benzoate	12158401	1
Caelo	Sodium benzoate	12158419	4
Fagron	Sodium benzoate	12J23-N05	3
Fagron	Sodium benzoate	13C14-N01	4
Caelo	Sodium benzoate	12158424	1
Noweda	Sodium benzoate	1209018-01	1
Caelo	Sodium benzoate	17061306	1
Caelo	Sodium benzoate	12J23-N05	1
Fiebig 27.06.13 EK3,34	Sodium benzoate	1304024-01	1
Caelo	Sodium benzoate	12158418	1
EuRho Anzag	Sodium benzoate	1304024-01	1
Euro OTC	Sodium benzoate	1304024-01	4
EuRho	Sodium benzoate	1112006-01	1
Caelo	Sodium benzoate	12158439	3
Alliance Healthcare	Sodium benzoate	1304024-01	1
Euro OTC	Sodium benzoate	130402401	2
Euro OTC	Sodium benzoate	2604040V-05	1
Caelo	Sodium benzoate	13178605	3
Caelo	Sodium benzoate	13178603	2
Fagron	Sodium benzoate	24011401	1
Caelo	Sodium benzoate	5211I-01891	1
Caelo	Sodium benzoate	13178613	1
Euro OTC	Sodium benzoate	1307013-01	2
Euro OTC	Sodium benzoate	1309027-01	1
Caelo	Sodium benzoate	13178619	2
Fagron	Sodium benzoate	13I27-B03288805	1
EuroTOC / Noweda	Sodium benzoate	130902701	1
Fagron	Sodium benzoate	13/27-B03-288805	1
Fagron	Sodium benzoate	13H01-N02	1
Caelo	Sodium benzoate	13178635	5
sana	Sodium benzoate	13178635	1
Fagron	Sodium benzoate	13C14-N01	1
Caelo	Sodium benzoate	13178627	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Sodium benzoate	1404011-01	4
Caelo	Sodium benzoate	13178647	2
Euro/ Phönix	Sodium benzoate	1404011-01	1
Fagron	Sodium benzoate	12H08-N06	1
Fagron	Sodium benzoate	13/27B03288805	1
Bombastus	Sodium benzoate	1404011-01	1
Fagron	Sodium benzoate	13127-B03-288806	1
Fagron	Sodium benzoate	13/27b03288805	1
Caelo	Sodium benzoate	24021501	1
Unisan	Sodium benzoate	1404011-01	1
Fagron	Sodium benzoate	13I27-B03-288806	3
Caelo	Sodium benzoate	15044102	5
Euro OTC	Sodium benzoate	1409040-01	1
Caelo	Sodium benzoate	14166714	1
Caelo	Sodium benzoate	14328702	1
Phoenix goettin	Sodium benzoate	13I27-B03-288806	1
Fagron	Sodium benzoate	14E12Bo7296717	1
Fagron	Sodium benzoate	14E12B07296717	1
Fagron	Sodium benzoate	14E12B07296717	1
Fagron	Sodium benzoate	14E12-B07-306570	1
Caelo	Sodium benzoate	1503022-01	1
Fagron	Sodium benzoate	14E12-B07	1
Fagron	Sodium benzoate	15B16-B07-306571	2
Caelo	Sodium benzoate	15044104	8
Euro OTC	Sodium benzoate	15060119-01	1
Caelo	Sodium benzoate	2215Q-01891	1
Caelo	Sodium benzoate	1506019-01	1
Euro OTC	Sodium benzoate	1506019-01	5
Fagron	Sodium benzoate	15B16-B07	1
Caelo	Sodium benzoate	15135001	5
Caelo	Sodium benzoate	15363401	8
Fagron	Sodium benzoate	1412	1
Euro OTC	Sodium benzoate	1602020-01	2
Fagron	Sodium benzoate	15363403	1
Euro OTC	Sodium benzoate	1510044-01	9
Caelo	Sodium benzoate	15363409	2
Hedinger	Sodium benzoate	13I27-B03	1
Fagron	Sodium benzoate	1602020-01	1
Caelo	Sodium benzoate	11346109	3
Caelo	Sodium benzoate	15363414	1
Caelo	Sodium benzoate	15363424	9
Caelo	Sodium benzoate	15363413	2
Phönix	Sodium benzoate	1510044/01	1
Caelo	Sodium benzoate	10544104	1
Caelo	Sodium benzoate	151208NB	1
Caelo	Sodium benzoate	91443209	2
Caelo	Sodium benzoate	4315A-01891	1
Hedinger/Phönix	Sodium benzoate	15363413	1
Caelo	Sodium benzoate	16137104	2
Euro OTC	Sodium benzoate	15363424	1
Caelo	Sodium benzoate	16137103	7
Caelo	Sodium benzoate	16137112	5
Caelo	Sodium benzoate	161371	1
Euro OTC	Sodium benzoate	1607005-01	2
Noweda	Sodium benzoate	16137103	1
Caelo	Sodium benzoate	17055801	5
Euro OCT / Noweda	Sodium benzoate	1510044-01	1
Caelo	Sodium benzoate	16137118	4
Caelo	Sodium benzoate	11267016	1
Euro OTC	Sodium benzoate	1610037-01	2

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Supplier	Substance	Batch	Spectra
Caelo	Sodium benzoate	1610037-01	1
Kehr	Sodium benzoate	1701045-01	1
Caelo	Sodium benzoate	18055805	1
Euro OTC	Sodium benzoate	1701045	1
Caelo	Sodium benzoate	17055805	3
Caelo	Sodium benzoate	17137604	3
Caelo	Sodium benzoate	5117A-01891	1
Caelo	Sodium benzoate	17137606	8
Bombastus	Sodium benzoate	17055805	1
AHD	Sodium benzoate	17137606	1
AHD	Sodium benzoate	1711019-01	3
Caelo	Sodium benzoate	17137609	1
Caelo	Sodium benzoate	NB20180313	1
Caelo	Sodium benzoate	17353001	2
Caelo	Sodium benzoate	17055806	1
Caelo	Sodium benzoate	17353002	1
calo	Sodium benzoate	17055805	1
Euro OTC	Sodium benzoate	1701045-01	1
Caelo	Sodium benzoate	19091801	1
Bombastus	Sodium benzoate	17353011	1
Caelo	Sodium benzoate	17353006	2
Nachtestung	Sodium benzoate	300/18	1
Caelo	Sodium benzoate	18161211	1

- 78 688 spectra from 565 *Apo-Ident* customers from a total of 26 035 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 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 *Sodium 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	360	0	74 136
Type B	0	440	0	126 452
Type C	0	241	0	78 688

The substance/substance group *Sodium 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 % (> 99.9887 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 97.5104 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22997	22997	0.00	30.93
22236	22236	0.00	27.94
21607	23900	6.99	26.06
21825	21825	0.00	24.33
20752	23900	7.71	26.64
23900	23900	0.00	34.38
22363	22363	0.00	29.39
21713	21825	7.37	30.16
22867	22867	0.00	30.26

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sodium citrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20662-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sodium citrate; Natrii citras

Special notes

When selecting the *Sodium citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sodium citrate	12E04-N05	20662	40	20120516
Caelo	Sodium citrate	12045026	20918	40	20120307
Caelo	Sodium citrate	13089335	21670	40	AR-15-FG-000405-01
Caelo	Sodium citrate	14112517	21718	40	20140416
Fagron	Sodium citrate	14A13-B02-294541	21778	40	20140424

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Sodium citrate	1506041	21839	40	0000010492
Euro OTC	Sodium citrate	1511017	21997	40	20151130*
Fagron	Sodium citrate	16F10-B01-326088	22843	40	20160711
Euro OTC	Sodium citrate	1610016	22859	40	20161102*
Euro OTC	Sodium citrate	1701029	22996	40	20170126*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Sodium citrate*. These samples are listed above in the [calibration samples](#) section.
- 74 096 spectra from a total of 1613 batches from further 372 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 [†].

- 460 spectra of 14 reference samples from the substance/substance group *Sodium citrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sodium citrate	1205026-01	20652	40
Caelo	Sodium citrate	12045008	20656	40
Caelo	Sodium citrate	13089335	21670 [†]	20
Caelo	Sodium citrate	14112517	21718 [†]	20
Fagron	Sodium citrate	14A13-B02-294541	21778 [†]	20
Euro OTC	Sodium citrate	1506041	21839 [†]	20
Euro OTC	Sodium citrate	1511017	21997 [†]	20
Euro OTC	Sodium citrate	1604030	22510	40
Caelo	Sodium citrate	162179	22618	40
Euro OTC	Sodium citrate	1607040	22687	40
Euro OTC	Sodium citrate	1710006	23614	40
Caelo	Sodium citrate	173236	23789	40
Euro OTC	Sodium citrate	1807035	24151	40
Caelo	Sodium citrate	182083	24218	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.

- 126 432 spectra from a total of 2775 batches from further 781 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.

- 828 spectra from 333 *Apo-Ident* customers from 215 batches from the substance/substance group *Sodium citrate*.

Supplier	Substance	Batch	Spectra
EuRho	Sodium citrate	1107011-02	1
Caelo	Sodium citrate	12045002	1
Caelo	Sodium citrate	11304311	3
Fagron	Sodium citrate	31051202	1
Caelo	Sodium citrate	12045004	3
Caelo	Sodium citrate	12045006	1
Fagron	Sodium citrate	12A05-N04	2
Caelo	Sodium citrate	12045008	4
Caelo	Sodium citrate	1234	3
Caelo	Sodium citrate	12045011	6
Fagron	Sodium citrate	12I10-N01	1
Caelo	Sodium citrate	12045001	1
EuRho	Sodium citrate	4611M-01900	1
EuRho	Sodium citrate	1205026-02	1
Caelo	Sodium citrate	21121203	1
Euro OTC	Sodium citrate	20200810-6	1
Fagron	Sodium citrate	3311E-01900	1
Euro OTC	Sodium citrate	1205026-02	4
Phönix	Sodium citrate	1205026-02	1
Caelo	Sodium citrate	12045016	5
Fagron	Sodium citrate	12J26-N02	2
Caelo	Sodium citrate	12045019	4
Caelo	Sodium citrate	1151351	2
Euro OTC	Sodium citrate	1107011-01	1
Noweda	Sodium citrate	11127001	1
Euro OTC	Sodium citrate	1413M-01900	1
Euro OTC	Sodium citrate	1211030-01	10
Phönix	Sodium citrate	12045019	1
Caelo	Sodium citrate	12045026	7
Caelo	Sodium citrate	12045024	5
Noweda	Sodium citrate	12045026	1
Phönix	Sodium citrate	12045024	1
Fagron	Sodium citrate	1234567	1
Fagron	Sodium citrate	712A-01900	1
Caelo	Sodium citrate	K-280313-1	1
Fagron	Sodium citrate	13A07-N01	6
Gehe	Sodium citrate	12045026	1
Caelo	Sodium citrate	4111Q-01900	1
Alliance Healthcare	Sodium citrate	1211030-01	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	Sodium citrate	12E04-N05	1
Caelo	Sodium citrate	25383143	1
Fagron	Sodium citrate	12339502	1
Caelo	Sodium citrate	13089304	2
Euro OTC	Sodium citrate	2903001-01	1
Test	Sodium citrate		1
Test	Sodium citrate	1234	1
Caelo	Sodium citrate	12045012	1
Fagron	Sodium citrate	1161207	3
Caelo	Sodium citrate		6
Caelo	Sodium citrate	13089308	7
Euro OTC	Sodium citrate	1305001-01	11
Sanacorp	Sodium citrate	13089308	1
Euro OTC	Sodium citrate	22101305	1
Europ Ots Pharma	Sodium citrate	13089304	1
HiperScan	Sodium citrate		1
Fagron	Sodium citrate	13B28-N02	5
Fagron	Sodium citrate	Probe	1
Euro OTC	Sodium citrate	30111301	1
Caelo	Sodium citrate	1308908	1
Caelo	Sodium citrate	12045016-3451311172	1
Euro/Phönix	Sodium citrate	1305001-01	1
Caelo	Sodium citrate	49131-01900	1
Caelo	Sodium citrate	11121303	1
Fagron	Sodium citrate	24121301	1
EuRho/Sanacorp	Sodium citrate	1107011-02	1
Caelo	Sodium citrate	1107011-01	1
Caelo	Sodium citrate	11219012	3
Euro OTC	Sodium citrate	1311035-01	23
Caelo	Sodium citrate	8/AKD41	1
Euro OTC	Sodium citrate	1107011-02	1
Caelo	Sodium citrate	70214PJK01	1
Caelo	Sodium citrate	13089317	7
Unisan	Sodium citrate	S/WReferenzUmstell	1
Euro OTC	Sodium citrate	1073240	1
Caelo	Sodium citrate	13089329	1
Caelo	Sodium citrate	13089325	3
Fagron	Sodium citrate	13D09-N01	4
Caelo	Sodium citrate	13089305	1
Caelo	Sodium citrate	13089331	5
Caelo	Sodium citrate	12897	1
Sanacorp	Sodium citrate	13089331	1
Caelo	Sodium citrate	123Test	5
Caelo	Sodium citrate	13089335	7
Caelo	Sodium citrate	131103501	1
Caesar & Loretz GmbH	Sodium citrate	13089334	1
Euro OTC	Sodium citrate	2114M1900	1
Caelo	Sodium citrate	14112502	19
Gehe 26.05.2014	Sodium citrate	13B28-N02	2
Caelo	Sodium citrate	1411502	1
Fagron	Sodium citrate	160614	1
Euro OTC	Sodium citrate	17061407	1
Caesar&Loretz GmbH	Sodium citrate	12045026	1
Sanacorp	Sodium citrate	1311035-01	1
Caelo	Sodium citrate	1161207	2
Caelo	Sodium citrate	13089319	4
Gehe	Sodium citrate	1311035-01	1
Euro OTC	Sodium citrate	1404033-01	12
Fagron	Sodium citrate	13089331	1
Caelo	Sodium citrate	13/24-B13-287921	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Sodium citrate	13I24-B13-287921	1
Euro OTC	Sodium citrate	1311025-01	1
Caelo	Sodium citrate	220914PML01	1
Fagron	Sodium citrate	13/24-B13-287921	3
Caelo	Sodium citrate	4680	1
Gatt-Koller	Sodium citrate	1073/04121412	1
Fargon/Alliance HC	Sodium citrate	13/24-B13-287921	1
Caelo	Sodium citrate	1404033-01	3
Caelo	Sodium citrate	1042	1
Euro OTC	Sodium citrate	140403301	4
Fagron	Sodium citrate	13A07-N01	1
Caelo	Sodium citrate	13089314	1
Fagron	Sodium citrate	14112502	2
Caelo	Sodium citrate	14112517	8
Caelo	Sodium citrate	14112520	1
Fagron	Sodium citrate	13I24-B13-287921	2
EuRho	Sodium citrate	140403301	1
Fagron	Sodium citrate	1172108	1
EuRho	Sodium citrate	1211030-01	1
Noweda	Sodium citrate	14A13-B02-294541	1
Caelo	Sodium citrate	14369402	3
Gehe/Euro	Sodium citrate	1412014-01	6
Gehe/Euro	Sodium citrate	1404033-01	2
Fagron	Sodium citrate	14A13-B02-294541	8
Fagron	Sodium citrate	1176767	3
EuRho	Sodium citrate	1412014-01	1
VDL;16.05.15;3,83EUR	Sodium citrate	14369406	1
Euro OTC	Sodium citrate	14201401	1
Caesar & Loretz GmbH	Sodium citrate	14369406	1
Euro OTC	Sodium citrate	1412014-01	15
Caelo	Sodium citrate	14369406	5
Fagron	Sodium citrate	14A13-B02-300395	4
Euro OTC	Sodium citrate	23062015C	1
Fagron	Sodium citrate	14A13b02300395	1
Caelo	Sodium citrate	123test	2
Caelo	Sodium citrate	1412014-01	1
Caelo	Sodium citrate	14369411	3
Caelo	Sodium citrate	1234Test	1
Caesar & Loretz GmbH	Sodium citrate	14112517	1
Caelo	Sodium citrate	14369413	13
Caelo	Sodium citrate	14369407	31
Fagron	Sodium citrate	13D09N01	1
Caelo	Sodium citrate	50815PMS01	1
Sanacorp	Sodium citrate	1436407	1
Caelo	Sodium citrate	11081514	1
Caelo	Sodium citrate	17081501	1
Euro OTC	Sodium citrate	1506041-01	15
Caesar&Loretz GmbH/Anzag	Sodium citrate	14369407	1
Bombastus	Sodium citrate	73155098	1
Caelo	Sodium citrate	Test	2
Caelo	Sodium citrate	14112518	1
EuRho/Sanacorp	Sodium citrate	1506041-01	1
Caelo	Sodium citrate	14369415	1
Euro OTC	Sodium citrate	1511017-01	26
Fagron	Sodium citrate	15C27-B01-309893	4
Caelo	Sodium citrate	1511017-01	3
Fagron	Sodium citrate	15C27-B01-312231	5
Caelo	Sodium citrate	2543	1
Euro OTC	Sodium citrate	151101701	1
Caelo	Sodium citrate	14369424	4

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Supplier	Substance	Batch	Spectra
Caelo	Sodium citrate	15C27-B01-309893	1
Phoenix	Sodium citrate	1511017-01	2
Caelo	Sodium citrate	140510/1	1
Caelo	Sodium citrate	2413A-01900	1
Caelo	Sodium citrate	123456789	1
Caelo	Sodium citrate	1123588946	1
Caelo	Sodium citrate	123456	1
Caelo	Sodium citrate	14369416	1
Caelo	Sodium citrate	14369423	9
Caelo	Sodium citrate	123658	1
Caelo	Sodium citrate	459842	1
Caelo	Sodium citrate	1256825	1
Phoenix	Sodium citrate	1506041-01	1
Caelo	Sodium citrate	14838	1
Caelo	Sodium citrate	14369414	1
Caelo	Sodium citrate	128896	1
Caelo	Sodium citrate	154662	1
Caelo	Sodium citrate	125874566	1
Fagron	Sodium citrate	815Q-01900	1
Euro OTC	Sodium citrate		4
Euro OTC	Sodium citrate	156422	1
Euro OTC	Sodium citrate	3454	1
Euro OTC	Sodium citrate	2546426	1
Euro OTC	Sodium citrate	1645265	3
Euro OTC	Sodium citrate	358528	1
Euro OTC	Sodium citrate	25425	2
Euro OTC	Sodium citrate	815757/6745	1
Euro OTC	Sodium citrate	12345	2
Caelo	Sodium citrate	TestmessungnachRep	1
Euro OTC	Sodium citrate	1521017-01	1
Fagron	Sodium citrate	1511017-01	1
Caesar&Loretz GmbH	Sodium citrate	14112502	1
EuRho / Phoenix	Sodium citrate	151101017-01	1
Fagron	Sodium citrate	15C27-B01-316106	1
Euro OTC	Sodium citrate	15111017-01	1
Caelo	Sodium citrate	16095702	3
Caelo	Sodium citrate	140731NC	1
Euro OTC	Sodium citrate	1607040-01	9
Euro OTC	Sodium citrate	160740-01	1
EuRho	Sodium citrate	1607040-01	5
Fagron	Sodium citrate	15c27-b01-321097	1
Fagron	Sodium citrate	15C27-B01-321097	1
Euro OTC	Sodium citrate	345678	1
Aug. Hedinger	Sodium citrate	8765456	1
Euro	Sodium citrate	1815M-01900	1
Caelo	Sodium citrate	2345678	1
Fagron	Sodium citrate	179915	2
Caelo	Sodium citrate	1607040-01	3
Euro OTC	Sodium citrate	16070-01	1
Fagron	Sodium citrate	15C27-B01-3211097	1
Caelo	Sodium citrate	2815A-01900	1
Euro OTC	Sodium citrate	3032805	2
Caelo	Sodium citrate	15212705	3
Fagron	Sodium citrate	16F10-B01-326088	1
Phoenix 30.05.2016	Sodium citrate	14369423	1
Euro OTC	Sodium citrate	1610016-01	27
Caelo	Sodium citrate	1610016-01	3
Caelo	Sodium citrate	16217901	1
Caelo	Sodium citrate	16217902	1
Fargon GmbH & Co.KG	Sodium citrate	16F10-B01-326088	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Sodium citrate	15212705	1
Caelo	Sodium citrate	16095707	5
Fagron	Sodium citrate	16F10-B01-327510	5
Fagron	Sodium citrate	15C27-B01-323451	1
Fagron	Sodium citrate	15C27	1
Caelo	Sodium citrate	16F10-B01-326093	1
Anzag	Sodium citrate	1512705	1
Euro/Phönix	Sodium citrate	1610016-01	1
Caelo	Sodium citrate	16217905	9
Fagron	Sodium citrate	1211142	2
Fagron	Sodium citrate	17A26-B04-331528	14
Noweda	Sodium citrate	16095707	1
Fagron	Sodium citrate	17A26-B04-331525	1
Euro OTC	Sodium citrate	1701029-01	16
Fagron	Sodium citrate	17A26-B04-332871	26
Caelo	Sodium citrate	16F10-B01-327510	1
GEHE	Sodium citrate	17A26-B04-332866	5
GEHE	Sodium citrate	17A26-B04-331525	6
AHD	Sodium citrate	1607040-01	2
Caelo	Sodium citrate	16217909	4
fargon	Sodium citrate	100772-114-91	1
Fagron	Sodium citrate	17A26-B04-335680	24
Caelo	Sodium citrate	171025NC/16217909	1
Caelo	Sodium citrate	1701029-01	3
Caelo	Sodium citrate	16217906	1
Caelo	Sodium citrate	16217908	1
AHD	Sodium citrate	1710006-01	2
Euro OTC	Sodium citrate	4716E-01900	1
Fagron	Sodium citrate	17H07-B04338530	28
EuRho	Sodium citrate	3032981	1
Fagron	Sodium citrate	17A26-B04-335883	1
EuRho	Sodium citrate	1070102901	1
Caelo	Sodium citrate	16217914	3
Caelo	Sodium citrate	16217912	2
Caelo	Sodium citrate	16217913	1
Sanacorp	Sodium citrate	17A26-B04-332866	1
Fagron	Sodium citrate	1190802	1
Unisan	Sodium citrate	1701029-01	1
Fagron	Sodium citrate	17H07-B04-341746	1
Noweda	Sodium citrate	1701029-01	1
Fagron	Sodium citrate	1219546	1
Sanacoro W.E:15.05.14 ...	Sodium citrate	14112502	1
Kehr	Sodium citrate	17A26-B04-331525	1
Caelo	Sodium citrate	17323601	11
Euro OTC	Sodium citrate	1710006-01	4
Noweda	Sodium citrate	3032981	1
Audor Pharma	Sodium citrate	171000601	1
Caelo	Sodium citrate	17H7-B04-345098	1
Fagron	Sodium citrate	17H07	1
Euro OTC	Sodium citrate	1701029-02	1
Caelo	Sodium citrate	1732361	1
AHD	Sodium citrate	17323602	1
Euro OTC	Sodium citrate	1710006-02	3
euro//Noweda	Sodium citrate	1701029-01	1
Caelo	Sodium citrate	17323609	1
Caelo	Sodium citrate	171006-02	1
Caelo	Sodium citrate	17323602	2
Caelo	Sodium citrate	17323608	7
Caelo	Sodium citrate	30081802	1
Fagron	Sodium citrate	18C05-B03	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Sodium citrate	1807035-01	5
Fagron	Sodium citrate	1807035-01	1
Caelo	Sodium citrate	17323612	1
Delta Apotheke	Sodium citrate	17323608	1
Caelo	Sodium citrate	1807035-01	1
Caelo	Sodium citrate	19121802	1
Fagron	Sodium citrate	18B14-B08-348067	1

- 78 101 spectra from 565 *Apo-Ident* customers from a total of 25 933 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 citrate* can clearly be 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 citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	400	0	74 096
Type B	0	460	0	126 432
Type C	0	823	5	78 101

The substance/substance group *Sodium citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.6957 %)
Type C	100.0000 % (> 99.8817 %)	99.3961 % (> 99.0338 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
20662	21839	3.99	41.67
22996	22996	0.00	37.67
21997	21997	0.00	42.63
21778	21670	3.84	43.40
21839	21839	0.00	41.96
21670	21670	0.00	44.34
20918	21670	5.22	44.07
22843	21839	5.20	43.59
21718	21670	3.25	43.99
22859	22859	0.00	32.25

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sodium cromoglicate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20775-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sodium cromoglicate; Natrii cromoglicas

Special notes

When selecting the *Sodium cromoglicate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 cromoglicate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sodium cromoglic...	12C09-N02	20775	79	1401553
Caelo	Sodium cromoglic...	11114501	20776	80	20110518
Fagron	Sodium cromoglic...	13G24-N04	21260	40	20130515
Caelo	Sodium cromoglic...	13232802	21375	20	1505352
Euro OTC	Sodium cromoglic...	1403017-01	21981	40	20140505

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium cromoglic...	15224404	21990	40	20150625
Euro OTC	Sodium cromoglic...	1510018	22231	40	20151109*
Euro OTC	Sodium cromoglic...	1703027	23383	40	20170405*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 379 spectra of 8 reference samples from the substance/substance group *Sodium cromoglicate*. These samples are listed above in the [calibration samples](#) section.
- 74 117 spectra from a total of 1615 batches from further 372 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 [†].

- 620 spectra of 14 reference samples from the substance/substance group *Sodium cromoglicate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sodium cromoglicate	1112003-01	20778	40
Caelo	Sodium cromoglicate	13232802	21376	110
Euro OTC	Sodium cromoglicate	1403017-01	21981 [†]	20
Caelo	Sodium cromoglicate	15224404	21990 [†]	20
Euro OTC	Sodium cromoglicate	1510018	22231 [†]	20
Fagron	Sodium cromoglicate	15C23-B01-307751	22972	40
Caelo	Sodium cromoglicate	173081	23855	30
Euro OTC	Sodium cromoglicate	1711024	23871	40
Caelo	Sodium cromoglicate	182657	24382	40
Euro OTC	Sodium cromoglicate	1811016	24424	40
Euro OTC	Sodium cromoglicate	1403017-01	21981SI	60
Caelo	Sodium cromoglicate	15224404	21990SI	60
Euro OTC	Sodium cromoglicate	1510018	22231SI	60
Fagron	Sodium cromoglicate	15C23-B01-307751	22972SI	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*.

- 126 272 spectra from a total of 2779 batches from further 781 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 8 *Apo-Ident* customers from 7 batches from the substance/substance group *Sodium cromoglicate*.

Supplier	Substance	Batch	Spectra
Caelo	Sodium cromoglicate	12301102	1
Fagron	Sodium cromoglicate	13E22-N11	1
Euro OTC	Sodium cromoglicate	1403017-01	1
Caelo	Sodium cromoglicate	5113A-02831	1
Bombastus	Sodium cromoglicate	15414502	1
Caelo	Sodium cromoglicate	15224404	1
Caelo	Sodium cromoglicate	16270705	2

- 78 921 spectra from 565 *Apo-Ident* customers from a total of 26 130 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 cromoglicate* can clearly be 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 cromoglicate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	365	14	74 117
Type B	0	593	27	126 272
Type C	0	6	2	78 921

The substance/substance group *Sodium cromoglicate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	96.3061 % (> 95.5145 %)
Type B	100.0000 % (> 99.9901 %)	95.6452 % (> 95.1613 %)
Type C	100.0000 % (> 99.8818 %)	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
20775	20775	0.00	69.64
20776	21375	20.38	74.19
21260	20775	8.48	70.60
21981	22231	17.39	73.40
21990	20775	16.71	74.69
22231	22231	0.00	73.61
23383	23383	0.00	70.51
21375	21375	0.00	80.64

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sodium cyclamate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20917-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sodium cyclamate; Natrii cyclamas

Special notes

When selecting the *Sodium cyclamate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 cyclamate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium cyclamate	12256803	20917	40	1401418
Caelo	Sodium cyclamate	12105622	21380	40	20120423
Caelo	Sodium cyclamate	182167	24379	40	20181023*

Validation samples

A total of 280 317 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 *Sodium cyclamate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Sodium cyclamate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium cyclamate	16119302	23259	40
Caelo	Sodium cyclamate	170411	23853	40

- 126 812 spectra from a total of 2787 batches from further 781 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 24 *Apo-Ident* customers from 13 batches from the substance/substance group *Sodium cyclamate*.

Supplier	Substance	Batch	Spectra
Caelo	Sodium cyclamate	10380915	2
Caesar & Loretz GmbH	Sodium cyclamate	12105622	1

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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
Caelo	Sodium cyclamate	11204205	1
Phoenix	Sodium cyclamate	787/03100611	1
Caelo	Sodium cyclamate	15201601	2
Caelo	Sodium cyclamate	15201606	2
Caelo	Sodium cyclamate	15201608	1
Caelo	Sodium cyclamate	15201614	1
Caelo	Sodium cyclamate	16119302	4
Caelo	Sodium cyclamate	16119302/2280217	1
Euro OTC	Sodium cyclamate	16119302	1
Caelo	Sodium cyclamate	16119308	3
Caelo	Sodium cyclamate	17041102	5
Caelo	Sodium cyclamate	17362202	4

- 78 900 spectra from 565 *Apo-Ident* customers from a total of 26 125 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 cyclamate* can clearly be 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 cyclamate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	80	0	126 812
Type C	0	29	0	78 900

The substance/substance group *Sodium cyclamate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 79.3103 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20917	20917	0.00	73.87
21380	20917	12.63	77.63
24379	24379	0.00	79.14

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sodium edetate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20937-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sodium edetate; Dinatrii edetas

Special notes

When selecting the *Sodium edetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 edetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sodium edetate	13E15-N05	20937	40	1402193
Caelo	Sodium edetate	13142009	21362	40	20130524
Caelo	Sodium edetate	161364	22465	40	20160504*
Euro OTC	Sodium edetate	1609023	22915	40	20170106*
Fagron	Sodium edetate	16F21-B02-325085	22926	40	20160713

Validation samples

A total of 280317 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 *Sodium edetate*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 8 reference samples from the substance/substance group *Sodium edetate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium edetate	161364	22465 [†]	20
Euro OTC	Sodium edetate	1609023-01	22950	40
Euro OTC	Sodium edetate	1704011	23390	40
Caelo	Sodium edetate	172618	23663	40
Caelo	Sodium edetate	172618	23818	40
Euro OTC	Sodium edetate	1806007	24157	40
Euro OTC	Sodium edetate	1807025	24159	40
Euro OTC	Sodium edetate	1812016	24414	40

- 126592 spectra from a total of 2782 batches from further 781 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.

- 338 spectra from 199 *Apo-Ident* customers from 109 batches from the substance/substance group *Sodium edetate*.

Supplier	Substance	Batch	Spectra
Phönix	Sodium edetate	11074702	1
Fagron	Sodium edetate	12E16-N04	2
Caelo	Sodium edetate	12181703	3
Fagron	Sodium edetate	601H1300	2
Caelo	Sodium edetate	3211I-01925	1
Sanacorp	Sodium edetate	12G25-N12	2
Caelo	Sodium edetate	11074703	1
Caelo	Sodium edetate	12181706	2
Caelo	Sodium edetate	12E16-N04	1
Fagron	Sodium edetate	813Q-01925	1
Caelo	Sodium edetate	12181704	1
Caesar & Loretz GmbH, 4...	Sodium edetate	12181711	1
Caelo	Sodium edetate	12181711	11
Caelo	Sodium edetate	92159379	1
Fagron	Sodium edetate	12G25-N12	3
Fagron	Sodium edetate	12E12-N04	1
Caelo	Sodium edetate	12181714	4
Cranach-Apotheke	Sodium edetate	11a31-no6	1
Alliance Healthcare	Sodium edetate	12181714	1
Fagron	Sodium edetate	12g25-n12	1
Fagron	Sodium edetate	13E15-N05	9
Caelo	Sodium edetate	13E15-N05	1
Caelo	Sodium edetate	12254507	1
Caelo	Sodium edetate	2913M1925	1
Noweda	Sodium edetate	601H1300	1
Caelo	Sodium edetate	13E15-N05	4
Alliance Healthcare	Sodium edetate	13E15-N05	2
Caelo	Sodium edetate	13142004	4
Phönix	Sodium edetate	13142004	1
Caelo	Sodium edetate	13142002	4
Gehe	Sodium edetate	13E15-N05	1
Fagron	Sodium edetate	601HA062	5
Caelo	Sodium edetate	13142008	6
Fagron	Sodium edetate	13I23-N03	10
Sanacorp	Sodium edetate	13E15-N05	1
Sanacorp	Sodium edetate	6/AKD14	1
Caelo	Sodium edetate	13/23-N03-3472312131	1
Fagron	Sodium edetate	13/23-N03	6
Caesar & Loretz GmbH	Sodium edetate	13142008	1
Fagron	Sodium edetate	5012Q-01925	1
Fagron	Sodium edetate	13G15-N03	4
Caelo	Sodium edetate	13142014	1
Fagron	Sodium edetate	13K19-B02-289035	1
Caelo	Sodium edetate	13142010	2
Fagron	Sodium edetate	13E15-B10-289034	1
Caelo	Sodium edetate	13142015	4
	Sodium edetate	13142009	1
Phönix	Sodium edetate	13E15-B10	1
Phönix	Sodium edetate	13G15-N03	1
Caelo	Sodium edetate	13142009	8
Caelo	Sodium edetate	12181702	1
Fagron	Sodium edetate	13I23-N03	1
Caelo	Sodium edetate	2101414	1
Fagron	Sodium edetate	13K19-B02-290051	7

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Supplier	Substance	Batch	Spectra
Caelo	Sodium edetate	13395002	3
Anzag	Sodium edetate	13K19-B02-290051	1
Fagron	Sodium edetate	914E-01925	1
Caelo	Sodium edetate	13395007	4
Phoenix Goettin	Sodium edetate	13G15-N03	1
Phoenix Goettin	Sodium edetate	13G15-N03	1
phönix	Sodium edetate	13142018	1
phönix	Sodium edetate	13K19-B02-290051	1
Fagron	Sodium edetate	13k19-b02-290051	2
Fagron	Sodium edetate	13K19B02290051	1
Fagron	Sodium edetate	13K19-B02-290052	3
Caelo	Sodium edetate	14270505	2
Caelo	Sodium edetate	14270506	3
Euro OTC	Sodium edetate	13142018	1
Caesar & Loretz GmbH	Sodium edetate	14270505	1
Caelo	Sodium edetate	13142018	2
Fagron	Sodium edetate	13K19-B02	1
Fagron	Sodium edetate	14G03-B05	4
Sanacorp	Sodium edetate	1505603	1
Fagron	Sodium edetate	13K19B02	1
Caelo	Sodium edetate	1427006	1
Caelo	Sodium edetate	15035604	4
Fagron	Sodium edetate	14G03-B05-30773	1
Caelo	Sodium edetate		1
Gehe	Sodium edetate	13142018	1
Caelo	Sodium edetate	15116603	12
Caelo	Sodium edetate	15035603	2
Fagron	Sodium edetate	11A31-N06Retest	1
Caelo	Sodium edetate	13K19-B02-290051	1
Caelo	Sodium edetate	11074608	2
Fagron	Sodium edetate	215I-01925	1
Fagron	Sodium edetate	14G03B05309971	1
Fagron	Sodium edetate	14G03-B05-309971	1
Fagron	Sodium edetate	14G03-B05-307737	6
Noweda/Gehe	Sodium edetate	14G03-B05-307737	1
Caelo	Sodium edetate	15427703	11
Caelo	Sodium edetate	15116602	4
phönix	Sodium edetate	15427703	1
Caelo	Sodium edetate	14G03-B05-307737	1
Phoenix	Sodium edetate	15427704	1
Caelo	Sodium edetate	15427704	2
Sanacorp 28.06.2016	Sodium edetate	15D01-B05-315877	1
Fagron	Sodium edetate	601EB174	1
Caelo	Sodium edetate	15427705	4
Caesar & Loretz GmbH	Sodium edetate	15427705	1
Fagron	Sodium edetate	14G03-B05307737	1
Euro OTC	Sodium edetate	15427703	1
Caelo	Sodium edetate	3913A-01925	1
sanacorp	Sodium edetate	16F21-B02-324370	1
phönix	Sodium edetate	15427704	1
Caelo	Sodium edetate	15427710	4
Fagron	Sodium edetate	14G03-B05-303420	1
Fagron	Sodium edetate	5315A-01925	1
Fagron	Sodium edetate	16F21-B02-324370	3
Caelo	Sodium edetate	15427714	20
Fagron	Sodium edetate	16F21-B02-325891	2
Caelo	Sodium edetate	15427717	8
Fagron	Sodium edetate	16F21-B02-327696	4
Bombastus	Sodium edetate		1
Fagron	Sodium edetate	16F21-B02-325085	3

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Supplier	Substance	Batch	Spectra
Caelo	Sodium edetate	1517E-01925	1
Caelo	Sodium edetate	16136404	3
Fagron	Sodium edetate	11A31-N06	1
Fagron	Sodium edetate	16f21-b02-327696	1
Fagron	Sodium edetate	16F21B02327696	1
Noweda	Sodium edetate	15427710	1
Caelo	Sodium edetate	16F21-B02-327696	1
Fagron	Sodium edetate	601EC350	1
Fagron	Sodium edetate	16F21-B02	1
Bombastus	Sodium edetate	16136404	1
Caelo	Sodium edetate	16337302	5
Fagron	Sodium edetate	16F21-B02-329900	1
Noweda	Sodium edetate	16337312	1
Fagron	Sodium edetate	16F21-B02-332039	1
Caelo	Sodium edetate	16337312	10
Fagron	Sodium edetate	17D25-B08-334827	2
Caelo	Sodium edetate	16337316	2
Fagron	Sodium edetate	17D25-B08-334827	1
Caelo	Sodium edetate	17336102	5
Fagron	Sodium edetate	17D25-B08	3
Caelo	Sodium edetate	14031801	1
Fagron	Sodium edetate	17D25-B08-338202	1
Fagron	Sodium edetate	601H9118	1
Fagron	Sodium edetate	17D25-B08-339881	1
Delta Apotheke	Sodium edetate	18007102	1
Fagron	Sodium edetate	18H03-B04-353034	2
Caelo	Sodium edetate	10887102	1
Fagron	Sodium edetate	18H03-B04-355280	1

- 78 591 spectra from 565 *Apo-Ident* customers from a total of 26 029 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 edetate* can clearly be 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 edetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	300	0	126 592
Type C	0	330	8	78 591

The substance/substance group *Sodium edetate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.8817 %)	97.6331 % (> 96.7456 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22926	22915	4.42	73.90
20937	20937	0.00	75.54
21362	22465	3.57	76.54
22465	22465	0.00	75.67
22915	22915	0.00	76.21

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Sodium methyl-4-hydroxybenzoate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	22602-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium methyl-4-hydroxybenzoate; Methylis parahydroxybenzoas natricus

Special notes

When selecting the *Sodium methyl-4-hydroxybenzoate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 methyl-4-hydroxybenzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium methyl-4-...	15358708	22602	40	AR-16-FG-015095-01
Caelo	Sodium methyl-4-...	15358713	23093	40	20151127
Caelo	Sodium methyl-4-...	170519	23289	40	20170308*

Validation samples

A total of 280 317 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 *Sodium methyl-4-hydroxybenzoate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Sodium methyl-4-hydroxybenzoate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium methyl-4-hydroxybenzo...	15358708	22603	40
Caelo	Sodium methyl-4-hydroxybenzo...	15358709	22776	40

- 126 812 spectra from a total of 2787 batches from further 781 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 *Sodium methyl-4-hydroxybenzoate*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded 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 *Sodium methyl-4-hydroxybenzoate* can clearly be 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 methyl-4-hydroxybenzoate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	80	0	126 812
Type C	0	0	0	78 929

The substance/substance group *Sodium methyl-4-hydroxybenzoate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8817 %)	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
23093	22602	5.91	49.59
23289	23289	0.00	48.29
22602	22602	0.00	48.43

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sodium salicylate, powdered**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21037-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sodium salicylate, powdered; Natrii salicylas plv.

Special notes

When selecting the *Sodium salicylate, powdered* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 salicylate, powdered*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium salicylat...	12158307	21037	40	1403225
Caelo	Sodium salicylat...	13140513	21689	40	20130531
Caelo	Sodium salicylat...	163053	23052	40	20161118*

Validation samples

A total of 280 317 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 *Sodium salicylate, powdered*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Sodium salicylate, powdered*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium salicylate, powdered	13140513	21689 [†]	20
Caelo	Sodium salicylate, powdered	16305301	22879	40

- 126 832 spectra from a total of 2787 batches from further 781 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 5 batches from the substance/substance group *Sodium salicylate, powdered*.

*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
Phoenix	Sodium salicylate, powdered	12158309	1
Caelo	Sodium salicylate, powdered	18061305	1
Fagron	Sodium salicylate, powdered	102091210	1
GATT-KOLLER/PHOENIX	Sodium salicylate, powdered	4853/11124512	1
Gehe	Sodium salicylate, powdered	13G31-B03-287961	1

- 78 924 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 salicylate, powdered* can clearly be 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 salicylate, powdered* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	60	0	126 832
Type C	0	3	2	78 924

The substance/substance group *Sodium salicylate, powdered* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.8819 %)	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
21037	21037	0.00	69.46
21689	21037	3.69	69.79
23052	23052	0.00	68.75

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Sodium tetraborate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20179-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium tetraborate; Borax

Special notes

When selecting the *Sodium tetraborate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 tetraborate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium tetraborate	13290118	21438	40	1412042
Euro OTC	Sodium tetraborate	1404025-01	21656	40	20140514
Euro OTC	Sodium tetraborate	1507024	21854	40	20150730*
Euro OTC	Sodium tetraborate	1510032	22235	40	20151118*
Caelo	Sodium tetraborate	161372	22475	40	20160624*
Euro OTC	Sodium tetraborate	1711002	23892	40	20171128*

Validation samples

A total of 280 317 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 *Sodium tetraborate*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 *Sodium tetraborate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium tetraborate	13290118	21438 [†]	20
Euro OTC	Sodium tetraborate	1404025-01	21656 [†]	20
Euro OTC	Sodium tetraborate	1507024	21854 [†]	20
Euro OTC	Sodium tetraborate	1510032	22235 [†]	20
Caelo	Sodium tetraborate	161372	22475 [†]	20
Euro OTC	Sodium tetraborate	1603043	22508	40
Caelo	Sodium tetraborate	161372	22621	40
Euro OTC	Sodium tetraborate	1607036	22713	40
Euro OTC	Sodium tetraborate	1701046	22990	40
Euro OTC	Sodium tetraborate	1804014	24093	40

- 126 592 spectra from a total of 2780 batches from further 781 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.

- 28 spectra from 21 *Apo-Ident* customers from 23 batches from the substance/substance group *Sodium tetraborate*.

Supplier	Substance	Batch	Spectra
Euro OTC	Sodium tetraborate	13111207	1
Fagron	Sodium tetraborate	12H09-N03	1
Euro OTC	Sodium tetraborate	1302034-01	1
Euro OTC	Sodium tetraborate	130203401	1
Caelo	Sodium tetraborate	11369431	1
Euro OTC	Sodium tetraborate	1309032-01	1
Caelo	Sodium tetraborate	1309032-01	1
Caelo	Sodium tetraborate	21051402	1
Borax Francais	Sodium tetraborate	1402002-01	1
Gatt-Koller / Phoenix	Sodium tetraborate	6187/01142114	1
Euro OTC	Sodium tetraborate	1408006-01	1
Caelo	Sodium tetraborate	13290118	1
Euro OTC	Sodium tetraborate	1503043-01	1
Caelo	Sodium tetraborate	14310905	2
Euro OTC	Sodium tetraborate	1507024-01	3
Phoenix	Sodium tetraborate	1603043-01	1
Euro OTC	Sodium tetraborate	160304301	1
Euro OTC	Sodium tetraborate	1607036-01	1
Caelo	Sodium tetraborate	16137201	1
Euro OTC	Sodium tetraborate	1701046-01	1
Euro OTC	Sodium tetraborate		1
Euro OTC	Sodium tetraborate	1711002-01	2
Sanacorp	Sodium tetraborate	171100201	1
Caelo	Sodium tetraborate	16081801	1

- 78 901 spectra from 565 *Apo-Ident* customers from a total of 26 115 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 tetraborate* can clearly be 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 tetraborate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	238	2	74 256
Type B	0	290	10	126 592
Type C	0	28	0	78 901

The substance/substance group *Sodium tetraborate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	99.1667 % (> 97.9167 %)
Type B	100.0000 % (> 99.9901 %)	96.6667 % (> 95.6667 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 78.5714 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21438	21438	0.00	44.31
21656	22475	4.98	46.52
21854	21854	0.00	42.92
22235	22235	0.00	41.68
22475	22475	0.00	45.15
23892	23892	0.00	35.01

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sorbic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20881-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sorbic acid; Acidum sorbicum

Special notes

When selecting the *Sorbic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Sorbic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sorbic acid	12038025	20881	40	20120315
Caelo	Sorbic acid	13334008	21460	40	AR-15-FG-007849-01
Caelo	Sorbic acid	14176214	22592	40	20140708
Caelo	Sorbic acid	15382002	22826	40	20151112
Caelo	Sorbic acid	162080	23859	40	20160722*

Validation samples

A total of 280 317 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 *Sorbic acid*. These samples are listed above in the [calibration samples](#) section.
- 74 296 spectra from a total of 1618 batches from further 372 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 *Sorbic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sorbic acid	13334008	21460 [†]	20
Caelo	Sorbic acid	14380714	22593	40
Caelo	Sorbic acid	162080	22616	40
Caelo	Sorbic acid	172056	23851	40
Caelo	Sorbic acid	182876	24384	40

- 126 712 spectra from a total of 2784 batches from further 781 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*.

- 241 spectra from 167 *Apo-Ident* customers from 60 batches from the substance/substance group *Sorbic acid*.

Supplier	Substance	Batch	Spectra
Caelo	Sorbic acid	29071201	1
Caelo	Sorbic acid	11203807	10
Finze	Sorbic acid	9280207	1
Caelo	Sorbic acid	11203806	2
Caelo	Sorbic acid	10305209	1
Caelo	Sorbic acid	9280207	1
Caelo	Sorbic acid	5012E-01048	1
Caelo	Sorbic acid	12038016	5
Phoenix	Sorbic acid	11203813	1
Anzag	Sorbic acid	12038016	1
Sanacorp	Sorbic acid	12038016	1
Caelo	Sorbic acid	12038020	4
Caelo	Sorbic acid	12038002	1
Noweda	Sorbic acid	12038016	1
Caelo	Sorbic acid	10305208	1
Caelo	Sorbic acid	12038012	1
Caelo	Sorbic acid	12330608	8
Caelo	Sorbic acid	11203812	1
Caelo	Sorbic acid	10120303	1
Noweda	Sorbic acid	12330608	1
Euro OTC	Sorbic acid	12038020	1
Caelo	Sorbic acid	12038025	1
Caelo	Sorbic acid	105505	1
Fagron	Sorbic acid	121394	1
Caelo	Sorbic acid	12330618	12
Caelo	Sorbic acid	4811Q-01048	1
Caelo	Sorbic acid	13334003	4
Phönix	Sorbic acid	12330618	1
Caelo	Sorbic acid	12038009	1
vdl 28.04.2014 preis:5,79	Sorbic acid		1
PHOENIX 12.05.2014	Sorbic acid	13334008	1
Sanacorp	Sorbic acid	13334008	1
Caelo	Sorbic acid	13334008	5
Gatt-Koller / Phoenix	Sorbic acid	2575/07142914	1
Caelo	Sorbic acid	13334010	7
Fagron	Sorbic acid	13334008	1
VDL;5,78EUR;18.12	Sorbic acid	14176206	1
Caelo	Sorbic acid	14176206	7
Fagron	Sorbic acid	14176206	1
Caelo	Sorbic acid	14176209	3
Caelo	Sorbic acid	14176207	1
Caelo	Sorbic acid	14176212	7
Caelo	Sorbic acid	14380702	3
Noweda	Sorbic acid	14176206	1
Caelo	Sorbic acid	14176214	8
Caelo	Sorbic acid	14176213	1
Caelo	Sorbic acid	14380704	1
Caelo	Sorbic acid	14380706	4
Caelo	Sorbic acid	14380713	2
Caelo	Sorbic acid	14380714	9
Caesar & Loretz/Noweda	Sorbic acid	14380706	1
Caelo	Sorbic acid	15382002	9
Noweda	Sorbic acid	14380706	1
Caelo	Sorbic acid	15382001	1
ALH	Sorbic acid	15382007	1
Caelo	Sorbic acid	15382007	3
Caelo	Sorbic acid	15382010	11

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Supplier	Substance	Batch	Spectra
phönix	Sorbic acid	15382010	1
Euro OTC	Sorbic acid	o216E-01048	1
Caelo	Sorbic acid	16208005	20
Caelo	Sorbic acid	1620808005	1
Caelo	Sorbic acid	170427AS/16208005	1
Caelo	Sorbic acid	28041726	1
Fischar	Sorbic acid	16208005	1
Caelo	Sorbic acid	16208009	9
Phönix	Sorbic acid	16208005	1
Caelo	Sorbic acid	16208012	5
Caelo	Sorbic acid	16208011	6
Gehe	Sorbic acid	16208011	1
Caelo	Sorbic acid	162080	1
Caelo	Sorbic acid	16208015	7
SanacorpWE: 23.09.14 E...	Sorbic acid	14176212	1
Caelo	Sorbic acid	16208016	3
Caelo	Sorbic acid	16208018	2
Caelo	Sorbic acid	16208020	5
Caelo	Sorbic acid	17343401	3
Caelo	Sorbic acid	162508016	1
Caelo	Sorbic acid	21041801	1
H.Lamotte	Sorbic acid	17343401	1
Caelo	Sorbic acid	17343411	4
Caelo	Sorbic acid	17343422	2
Caesar & Loretz GmbH	Sorbic acid	18287605	1
Caelo	Sorbic acid	18287605	1

- 78 688 spectra from 565 *Apo-Ident* customers from a total of 26 077 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sorbic 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 *Sorbic 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	200	0	74 296
Type B	0	180	0	126 712
Type C	0	202	39	78 688

The substance/substance group *Sorbic 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 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.8817 %)	83.8174 % (> 82.5726 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20881	23859	3.04	49.27
21460	21460	0.00	48.82
22592	23859	2.45	49.55
22826	23859	5.39	48.60
23859	23859	0.00	48.86

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sorbitol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20075-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sorbitol; Sorbitolum

Special notes

When selecting the *Sorbitol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Sorbitol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sorbitol	13278217	21485	40	20130920
Euro OTC	Sorbitol	1506052	21834	40	20150713*
Euro OTC	Sorbitol	1512016	22293	40	20160113*
Euro OTC	Sorbitol	1604007	22539	40	20160428*
Caelo	Sorbitol	16038501	22847	40	20160315
Euro OTC	Sorbitol	1610018	22849	40	20161121*

Validation samples

A total of 280 317 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 *Sorbitol*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 *Sorbitol*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sorbitol	1506052	21834 [†]	20
Euro OTC	Sorbitol	1512016	22293 [†]	20
Caelo	Sorbitol	163531	23028	40
Caelo	Sorbitol	16353107	23442	40
Caelo	Sorbitol	181636	24220	40
Euro OTC	Sorbitol	1810010	24306	40

- 126 692 spectra from a total of 2783 batches from further 781 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*.

- 178 spectra from 63 *Apo-Ident* customers from 97 batches from the substance/substance group *Sorbitol*.

Supplier	Substance	Batch	Spectra
Caelo	Sorbitol	10383323	1
Caelo	Sorbitol		1
Fagron	Sorbitol	11I09-N11	1
Caelo	Sorbitol	12345	1
Caelo	Sorbitol	23071201	1
Fagron	Sorbitol	12E30-N24	3
Caelo	Sorbitol	17011305	1
Caelo	Sorbitol	11379332	2
Caelo	Sorbitol	11379321	1
Caelo	Sorbitol	5021307	1
Caelo	Sorbitol	11379337	2
Caelo	Sorbitol	1083330	1
Caelo	Sorbitol	11379322	1
Caelo	Sorbitol	12249108	2
Fagron	Sorbitol	12J15-N01	1
Fagron	Sorbitol	12L17-N12	3
Caelo	Sorbitol	11379336	2
Caelo	Sorbitol	12249110	4
Euro OTC	Sorbitol	1301019-01	3
Caelo	Sorbitol	12249124	2
Fagron	Sorbitol	M721140/12L17-N12	1
Caelo	Sorbitol	12L07-N12	1
Caelo	Sorbitol	12249126	2
Caelo	Sorbitol	16101303	1
Caelo	Sorbitol	12249109	1
Caelo	Sorbitol	12249139	1
Gatt-Koller / Phoenix	Sorbitol	1718/0513	1
Bombastus	Sorbitol	13278206	2
Caelo	Sorbitol	13335304	1
Caelo	Sorbitol	13335307	3
Caelo	Sorbitol	12249140	1
Caelo	Sorbitol	13278206	1
Fagron	Sorbitol	13D08-N27	1
Merck	Sorbitol	13D08-N27	1
Fagron	Sorbitol		1
Caelo	Sorbitol	13278204	1
Fagron	Sorbitol	13E07-B40	2
Phoenix 12.08.2013	Sorbitol	12249108	1
Caelo	Sorbitol	133335307	1
Fagron	Sorbitol	13G04-N04	1
Fagron	Sorbitol	M721140	1
Caelo	Sorbitol	13278216	2
Gatt-Koller / Phoenix	Sorbitol	1718/05134013	1
Caelo	Sorbitol	26071402	1
Caelo	Sorbitol	23081401	1
Caelo	Sorbitol	8081402	1
Gehe 01.09.2014	Sorbitol	13278217	1
Caelo	Sorbitol	4091401	1
Caelo	Sorbitol	13278218	1
Euro OTC	Sorbitol	1311034-01	1
Caelo	Sorbitol	13278247	1
Euro OTC	Sorbitol	1404007-01	2
Caelo	Sorbitol	13278239	1
GEHE 28.11.2014	Sorbitol	13278245	1
Caelo	Sorbitol	13278246	2
Euro OTC	Sorbitol	700476	1

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Supplier	Substance	Batch	Spectra
Caelo	Sorbitol	13278249	1
Fagron	Sorbitol	13278249	1
Caelo	Sorbitol	13278241	1
Caelo	Sorbitol	20021501	1
Caelo	Sorbitol	14250807	1
Fagron	Sorbitol	14E21-B02	1
Euro OTC	Sorbitol	1406014-01	1
Caelo	Sorbitol	13278250	1
Caelo	Sorbitol	14250808	1
Euro OTC	Sorbitol	1501048-01	3
Caelo	Sorbitol	14250806	1
Caelo	Sorbitol	15118902	2
Caelo	Sorbitol	15118901	3
Euro OTC	Sorbitol	1506052-01	4
Euro OTC	Sorbitol	150652-01	1
Caelo	Sorbitol	15208302	4
Caelo	Sorbitol	15208303	1
Caelo	Sorbitol	15208306	2
Caelo	Sorbitol	15012708	1
Caelo	Sorbitol	15208305	3
Caelo	Sorbitol	15208309	3
Caelo	Sorbitol	1512016-01	2
Euro OTC	Sorbitol	1512016-01	1
Caelo	Sorbitol	15208311	2
EuRho/Anzag	Sorbitol	4712I-02298	1
Caelo	Sorbitol	16038501	4
Euro OTC	Sorbitol	1604007-01	4
Caelo	Sorbitol	16038502	1
Noweda/ Ichthyol	Sorbitol	1512016-01	1
Caelo	Sorbitol	15208310	3
Caelo	Sorbitol	16038503	1
Caelo	Sorbitol	15118912	1
Caelo	Sorbitol	1604007-01	1
Caelo	Sorbitol	16038515	5
eurho	Sorbitol	1301019-01	1
siehe Protokoll	Sorbitol	15208310	1
Caelo	Sorbitol	16353102	3
Euro OTC	Sorbitol	1610018-01	10
Caelo	Sorbitol	16038514	4
Caelo	Sorbitol	16231208	1
Caelo	Sorbitol	1714090903	1
Caelo	Sorbitol	17140903	5
Caelo	Sorbitol	17140902	1
EuRho	Sorbitol	161001802	1
Caelo	Sorbitol	17140904	1
Euro OTC	Sorbitol	1610018-02	1
Caelo	Sorbitol	11379333	1
Caelo	Sorbitol	17366301	1
Caelo	Sorbitol	17366304	1
Euro OTC	Sorbitol	1610018-03	1
Caelo	Sorbitol	18163606	2

- 78 751 spectra from 565 *Apo-Ident* customers from a total of 26 045 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sorbitol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sorbitol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	200	0	126 692
Type C	0	174	4	78 751

The substance/substance group *Sorbitol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8817 %)	97.7528 % (> 96.0674 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21834	21834	0.00	40.11
22293	22293	0.00	40.08
22539	22539	0.00	38.37
22849	22849	0.00	37.90
21485	22539	3.69	41.84
22847	21834	2.08	41.09

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Soy lecithin (instant form)
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20539-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Soy lecithin (instant form); Lecithinum e sojae plv.

Special notes

When selecting the *Soy lecithin (instant form)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Soy lecithin (instant form)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Soy lecithin (in...	13030504	20985	40	1404399
Caelo	Soy lecithin (in...	13279813	21523	40	20130903
Caelo	Soy lecithin (in...	17118101	23370	40	20170620

Validation samples

A total of 280 317 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 *Soy lecithin (instant form)*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Soy lecithin (instant form)*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Soy lecithin (instant form)	17118101	23445	40
Caelo	Soy lecithin (instant form)	173224	24244	40

- 126 812 spectra from a total of 2787 batches from further 781 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 24 *Apo-Ident* customers from 25 batches from the substance/substance group *Soy lecithin (instant form)*.

Supplier	Substance	Batch	Spectra
Caelo	Soy lecithin (instant form)	12139001	3
Caelo	Soy lecithin (instant form)	11371504	1
Caelo	Soy lecithin (instant form)	12139011	3
Caelo	Soy lecithin (instant form)		1

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Supplier	Substance	Batch	Spectra
Caelo	Soy lecithin (instant form)	12139012	1
Caesar & Loretz GmbH, 4. ...	Soy lecithin (instant form)	12139013	1
Caelo	Soy lecithin (instant form)	13030503	1
Caesar & Loretz GmbH	Soy lecithin (instant form)	13030503	1
siehe WE-Prüfprotokoll	Soy lecithin (instant form)	31/14	1
Caelo	Soy lecithin (instant form)	13279806	1
Caelo	Soy lecithin (instant form)	13279814	1
Caesar & Loretz GmbH	Soy lecithin (instant form)	13279813	1
Sanacorp	Soy lecithin (instant form)	14196305	1
Caelo	Soy lecithin (instant form)	14281605	1
Caelo	Soy lecithin (instant form)	14281606	1
Caelo	Soy lecithin (instant form)	14281620	1
Caelo	Soy lecithin (instant form)	14281618	4
Caelo	Soy lecithin (instant form)	14196305	1
Caelo	Soy lecithin (instant form)	15262701	4
Caesar & Loretz GmbH	Soy lecithin (instant form)	14281603	1
Caelo	Soy lecithin (instant form)	1526704	1
Caelo	Soy lecithin (instant form)	16223302	1
INTR/ Sana	Soy lecithin (instant form)	16223302	1
Caelo	Soy lecithin (instant form)	17081501	1
Caelo	Soy lecithin (instant form)	17118101	1
Caelo	Soy lecithin (instant form)	17118108	1
Caelo	Soy lecithin (instant form)	17322401	1
Sanacorp	Soy lecithin (instant form)	17322405	1

- 78 891 spectra from 565 *Apo-Ident* customers from a total of 26 114 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Soy lecithin (instant form)* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Soy lecithin (instant form)* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	80	0	126 812
Type C	0	36	2	78 891

The substance/substance group *Soy lecithin (instant form)* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.8817 %)	94.7368 % (> 86.8421 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20985	20985	0.00	46.57
21523	20985	11.84	49.86
23370	20985	7.32	48.59

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Spironolactone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21032-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Spironolactone; Spironolactonum

Special notes

When selecting the *Spironolactone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Spironolactone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Spironolactone	1212034-01	21032	50	1403151
Euro OTC	Spironolactone	1602006	22369	30	20160309*
Caelo	Spironolactone	14378715	22385	40	20150211
Fagron	Spironolactone	2294216E20-B06-322016	22942	40	20160531

Validation samples

A total of 280 317 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 *Spironolactone*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 [†].

- 437 spectra of 11 reference samples from the substance/substance group *Spironolactone*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Spironolactone	1212034-01	21076	42
Euro OTC	Spironolactone	1602006	22369 [†]	15
Fagron	Spironolactone	15G22-B10-311159	22386	40
Caelo	Spironolactone	160773	22444	60
Euro OTC	Spironolactone	1612002	22909	40
Caelo	Spironolactone	16077305	22954	40
Caelo	Spironolactone	171165	23327	40
Caelo	Spironolactone	172432	23660	40
Euro OTC	Spironolactone	1711013	23888	40
Euro OTC	Spironolactone	1809020	24324	40
Caelo	Spironolactone	182080	24391	40

- 126 455 spectra from a total of 2778 batches from further 781 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.

- 254 spectra from 114 *Apo-Ident* customers from 101 batches from the substance/substance group *Spironolactone*.

Supplier	Substance	Batch	Spectra
Euro OTC	Spironolactone	1101013-01	1
Euro OTC	Spironolactone	1004035	1
EuRho	Spironolactone	1101013-01	1
Noweda	Spironolactone	1101013-0	1
Gehe	Spironolactone	12049105	1
Caelo	Spironolactone	11042607	1
Fagron	Spironolactone	12I17-N01	1
Sanacorp	Spironolactone	11042612	1
Sanacorp	Spironolactone	12049103	2
Caelo	Spironolactone	12049103	1
Caelo	Spironolactone	12049105	2
Caelo	Spironolactone	12049109	1
Caelo	Spironolactone	11G28-N03	1
Caesar&lorenz,Phoenix	Spironolactone	11042613	1
Fagron	Spironolactone	12/17-n01	1
Fagron	Spironolactone	12J15-N04	1
Caelo	Spironolactone	10159914	1
Caelo	Spironolactone	2013U-03249	1
Caelo	Spironolactone	11042602	1
Caelo	Spironolactone	12049118	2
Caelo	Spironolactone	12049110	2
Caesar&lorenz,Phoenix	Spironolactone	11042603	1
Phönix	Spironolactone	1101013-03	1
Euro OTC	Spironolactone	1212034-01	3
Euro OTC	Spironolactone	3513E-03249	1
Caesar u Lorenz	Spironolactone	12049119	1
Caelo	Spironolactone	13124303	7
Caesar & Lorenz GmbH	Spironolactone	12049129	1
Alliance Healthcare	Spironolactone	12049129	1
Fagron	Spironolactone	10H24-N10	2
Caelo	Spironolactone	12049123	3
Alliance Healthcare	Spironolactone	12049119	1
Fagron	Spironolactone	12/17-N01	1
Caelo	Spironolactone	12049130	4
Sanacorp	Spironolactone	12049130	1
Caesar/Lorenz	Spironolactone	13124303	1
Fagron	Spironolactone	13G03-N09	1
Caelo	Spironolactone	13124304	7
Caelo	Spironolactone	13124309	2
Caelo	Spironolactone	1314309	1
Caesar&lorenz,Anzag	Spironolactone	13124309	1
Sanacorp/Phoenix	Spironolactone	13124315	3
Fagron	Spironolactone	13G16-B08-288051	1
Caelo	Spironolactone	13124315	5
Caelo	Spironolactone	13124317	3
Fagron	Spironolactone	13D12-N08	1
Caelo	Spironolactone	5013Q-03249	1
Caelo	Spironolactone	140202901	1
Sanacorp	Spironolactone	1212034-01	1
Caelo	Spironolactone	13124314	2
Fagron	Spironolactone	14B20-B06-294618	5
Euro OTC	Spironolactone	1402029-01	1

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Supplier	Substance	Batch	Spectra
Caelo	Spironolactone	13124321	2
Caelo	Spironolactone	13190309	1
Caelo	Spironolactone	13124320	3
Fagron	Spironolactone	14B20B06294618	1
Caelo	Spironolactone	14378702	1
Fagron	Spironolactone	14J02-B02-303621	5
Euro OTC	Spironolactone	1504016-01	1
Fagron	Spironolactone	14J02-B303621	1
Caelo	Spironolactone	14378710	2
Caelo	Spironolactone	14378709	3
Noweda	Spironolactone	14378710	1
Caelo	Spironolactone	14378703	1
Caelo	Spironolactone	1437807	1
Caelo	Spironolactone	14378717	2
Fagron	Spironolactone	14j02-b02-303621	1
Caelo	Spironolactone	14378715	4
Caelo	Spironolactone	14378718	6
Jenne	Spironolactone	14378715	1
Fagron	Spironolactone	80616-7	1
Fagron	Spironolactone	2415E-03249	1
Caelo	Spironolactone	14378721	2
Caelo	Spironolactone	16077302	9
Caelo	Spironolactone	14378719	1
Caelo	Spironolactone	1438721	1
Fagron	Spironolactone	16A14-B05-317123	1
Caelo	Spironolactone		1
Caelo	Spironolactone	16077303	10
Caelo	Spironolactone	160773	1
Caelo	Spironolactone	14378701	2
Caelo	Spironolactone	15G22-B10	1
Caelo	Spironolactone	16077306	3
WE Phönix 25.11..2016 ...	Spironolactone	16077303	1
Fagron	Spironolactone	16D15-B06-320903	1
Caelo	Spironolactone	16077305	4
Fagron	Spironolactone	16A14-B05-525187	1
Caelo	Spironolactone	16077307	1
Caelo	Spironolactone	16077309	4
Fagron	Spironolactone	16E20-B06-325478	1
Caelo	Spironolactone	16077311	10
Fagron	Spironolactone	16E20-B06-322016	1
Caelo	Spironolactone	16D15-B06-320903	1
Fagron	Spironolactone	16I06-B04	1
Noweda	Spironolactone	1504016-01	1
Caelo	Spironolactone	16077312	6
Euro OTC	Spironolactone	1612002-01	2
Noweda	Spironolactone	1602006-01	1
Caelo	Spironolactone	17116501	1
Caelo	Spironolactone	16077319	4
Caelo	Spironolactone	16077320	5
Noweda	Spironolactone	1612002-01	1
Euro OTC	Spironolactone	16020006-01	1
Caelo	Spironolactone	17116502	6
gehe	Spironolactone	17E22-B11-335455	1
Caelo	Spironolactone	16077324	1
Fagron	Spironolactone	17116502	1
Caelo	Spironolactone	16077326	4
Euro OTC	Spironolactone	1711013-01	1
Fagron	Spironolactone	17H16-B05	2
GEHE	Spironolactone	16077325	1
Caelo	Spironolactone	16077325	5

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Supplier	Substance	Batch	Spectra
Caelo	Spironolactone	18004803	5
Caelo	Spironolactone	18004904	3
Caelo	Spironolactone	18004908	3
Cealo/Gehe	Spironolactone	18004904	2
Sanacorp	Spironolactone	18004913	1
Fagron	Spironolactone	17H16-B05-344771	1
Caelo	Spironolactone	18004917	5
Caelo	Spironolactone	18004915	3

- 78 675 spectra from 565 *Apo-Ident* customers from a total of 26 037 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Spironolactone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Spironolactone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	437	0	126 455
Type C	0	239	15	78 675

The substance/substance group *Spironolactone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.6270 %)
Type C	100.0000 % (> 99.8817 %)	94.0945 % (> 92.9134 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21032	21032	0.00	45.97
22942	22369	3.47	43.84
22369	22369	0.00	45.67
22385	22369	5.80	45.91

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Spray-dried arabic gum**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20457-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Spray-dried arabic gum; Acaciae gummi dispersione desiccatum

Special notes

When selecting the *Spray-dried arabic gum* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Spray-dried arabic gum*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Spray-dried arab...	14141901	21431	80	AR-15-FG-006809-01
Caelo	Spray-dried arab...	15413201	22653	40	AR-17-FG-000844-01

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 2 reference samples from the substance/substance group *Spray-dried arabic gum*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1621 batches from further 372 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 *Spray-dried arabic gum*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Spray-dried arabic gum	14141901	21431 [†]	40
Caelo	Spray-dried arabic gum	162331	22853	40
Caelo	Spray-dried arabic gum	16233105	23443	40
Caelo	Spray-dried arabic gum	16233105	23444	40

- 126732 spectra from a total of 2786 batches from further 781 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.

- 10 spectra from 8 *Apo-Ident* customers from 10 batches from the substance/substance group *Spray-dried arabic gum*.

Supplier	Substance	Batch	Spectra
Caelo	Spray-dried arabic gum	11345715	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	Spray-dried arabic gum	12138607	1
Caelo	Spray-dried arabic gum	12372302	1
Caelo	Spray-dried arabic gum	12138612	1
Klenk	Spray-dried arabic gum	3314A140121	1
Caelo	Spray-dried arabic gum	12111301	1
Caelo	Spray-dried arabic gum	15413201	1
Caelo	Spray-dried arabic gum	15086704	1
Caelo	Spray-dried arabic gum	15413207	1
Caelo	Spray-dried arabic gum	3314A160121	1

- 78 919 spectra from 565 *Apo-Ident* customers from a total of 26 127 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Spray-dried arabic gum* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Spray-dried arabic gum* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	0	126 732
Type C	0	8	2	78 919

The substance/substance group *Spray-dried arabic gum* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8818 %)	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
21431	21431	0.00	12.00
22653	22653	0.00	16.13

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Starch**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20790-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Starch; Amylum Maydis; Amylum oryzae; Amylum Solani; Amylum tritici; Corn starch; Potato starch; Rice starch; Wheat starch

Special notes

When selecting the *Starch* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Starch*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Rice starch	12068525	20790	40	20120327
Caelo	Potato starch	12360213	20996	40	1403494
Caelo	Wheat starch	14023203	21447	40	AR-16-FG-011433-01
Caelo	Corn starch	13154914	21827	40	20130529

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potato starch	14033815	21965	40	20140207
Klenk	Wheat starch	0104A141114	21973	40	20141210
Caelo	Wheat starch	15124707	22246	40	20150527
Caelo	Potato starch	161237	22449	40	20160621*
Caelo	Corn starch	161385	22450	40	20160621*
Caelo	Rice starch	16144501	22585	40	20160504
Caelo	Rice starch	162180	22642	40	20160901*
Fagron	Rice starch	16B25-B01-327231	23220	40	AR-17-FG-015298-02
Klenk	Potato starch	0094A170123	23923	40	20170309
Caelo	Corn starch	182748	24361	40	20181031*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 560 spectra of 14 reference samples from the substance/substance group *Starch*. These samples are listed above in the [calibration samples](#) section.
- 73 936 spectra from a total of 1609 batches from further 369 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 [†].

- 500 spectra of 16 reference samples from the substance/substance group *Starch*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Wheat starch	14023203	21447 [†]	20
Caelo	Corn starch	13154914	21827 [†]	20
Caelo	Potato starch	14033815	21965 [†]	20
Klenk	Wheat starch	0104A141114	21973 [†]	20
Caelo	Wheat starch	15124707	22246 [†]	20
Caelo	Potato starch	161237	22449 [†]	20
Caelo	Corn starch	161385	22450 [†]	20
Caelo	Potato starch	15062921	23189	40
Caelo	Corn starch	16138505	23217	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
Fagron	Rice starch	16B25-B01-327231	23219	40
Caelo	Wheat starch	15421507	23509	40
Klenk	Wheat starch	0104A160512	23510	40
Caelo	Potato starch	173003	23811	40
Caelo	Corn starch	172873	23813	40
Caelo	Wheat starch	181200	24014	40
Caelo	Corn starch	170474	24037	40

- 126 392 spectra from a total of 2773 batches from further 778 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.

- 200 spectra from 113 *Apo-Ident* customers from 83 batches from the substance/substance group *Starch*.

Supplier	Substance	Batch	Spectra
Caelo	Rice starch	10177507	1
Caelo	Rice starch	10177515	1
Caelo	Rice starch	12214303	1
Caelo	Rice starch	11132406	1
Caelo	Rice starch	12166007	3
Caelo	Rice starch	9352108	1
Klenk	Rice starch	64A130304	12
Klenk	Rice starch	104A120621	4
Caelo	Rice starch	12238714	1
Klenk	Rice starch	64A080218	1
Koisser	Rice starch	WE07032013	1
Fagron	Rice starch	12L19-N06	1
Caelo	Rice starch	104A120621	1
Caelo	Rice starch	13154904	2
Caelo	Rice starch	11186026	1
Nachprüfung	Rice starch	3709E01116	1
Caelo	Rice starch	10061134	2
Caelo	Rice starch	13005905	2
Klenk	Rice starch	84A130304	1
Caelo	Rice starch	13154914	1
Klenk	Rice starch	94A100122	1
Caelo	Rice starch	200613K3	1
Caelo	Rice starch	14025710	1
Klenk	Rice starch	104A130304	7
Caelo	Rice starch	13005908	1
Caelo	Rice starch	13305103	3
Caelo	Rice starch	13305108	1
Gutenberg-Apotheke	Rice starch	12360216	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	Rice starch	14011612	3
Cealo	Rice starch	13305103	1
Noweda	Rice starch	14023203	1
Caelo	Rice starch	2212M-01115	1
sanacorp	Rice starch	94A130304	1
Caelo	Rice starch	14023203	3
Caelo	Rice starch	16101401	1
Caelo	Rice starch	14011621	1
Noweda	Rice starch	14011621	1
Klenk	Rice starch	64a130304	1
Caelo	Rice starch	12238719	1
VDL;03.03.15;3,04EUR	Rice starch	14011627	1
Caelo	Rice starch	14011630	2
Klenk	Rice starch	104A141114	3
Klenk	Rice starch	94A130304	2
Fagron	Rice starch	14F18-B04-301616	1
VDL;3,03EUR;11.06.15	Rice starch	14011630	1
Caelo	Rice starch	64A130304	1
Caelo	Rice starch	14025733	1
Caelo	Rice starch	104A141114	1
Caelo	Rice starch	15118607	1
Caelo	Rice starch	14301214	1
Klenk	Rice starch	84A141114	3
Caelo	Rice starch	15119011	1
Caelo	Rice starch	16218002	1
phönix	Rice starch	84a141114	1
Euro OTC	Rice starch	17173501	2
Caelo	Rice starch	16218009	1
Caelo	Rice starch	17327503	2
Caelo	Rice starch	17327502	1
Sanacorp	Rice starch	84A141114	1
Caelo	Corn starch	11179307	2
Klenk	Corn starch	64A080218	4
Caelo	Corn starch	10061146	1
Caelo	Corn starch	12238705	1
Caelo	Corn starch	12238715	2
Caelo	Corn starch	15119011	5
Caelo	Corn starch	13154904	1
Klenk	Corn starch	64A130304	5
Caelo	Corn starch	13154914	1
Fagron	Corn starch	15310902	1
Caelo	Corn starch	15310902	1
Caelo	Corn starch	15310903	2
Caelo	Corn starch	64A130304	2
Caelo	Corn starch	15310914	4
Caelo	Corn starch	15310909	2
Caelo	Corn starch	15310904	1
Caelo	Corn starch	16138505	4
Caelo	Corn starch	16138507	2
Klenk	Corn starch	64A170123	4
Caelo	Corn starch	14111701	1
Caelo	Corn starch	17047404	5
Cealo/Sanacorp	Corn starch	17287302	1
Caelo	Corn starch	17287302	1
Klenk	Wheat starch	104A101116	1
Caelo	Wheat starch	11350907	1
Caelo	Wheat starch	1114611	1
Fiebig 16.01.13 ek: 4,18EUR	Wheat starch	11350911	1
Anzag 05.03.13 ek: 9,65EUR	Wheat starch	104A120621	2
Caelo	Wheat starch	11350911	2

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Supplier	Substance	Batch	Spectra
Klenk	Wheat starch	104A120621	1
Fresenius	Wheat starch	13305103	1
Klenk	Wheat starch	104a141114	1
Klenk	Wheat starch	104A141114	5
Caelo	Wheat starch	104A141114	2
Caelo	Wheat starch	1512477	1
Caelo	Wheat starch	15124707	1
Klenk	Wheat starch	10A160512	1
Klenk	Wheat starch	104A160512	8
Caelo	Wheat starch	15421507	1
Klosterring	Wheat starch	15421507	1
Klenk	Wheat starch	104A171122	1
Kehr	Wheat starch	104A160512	1
Caelo	Potato starch	11301012	2
Klenk	Potato starch	94A110512	1
Bombastus	Potato starch	12214303	2
Caelo	Potato starch	14033815	1
Klenk	Potato starch	94A130304	3
Caelo	Potato starch	15062912	2
Klenk	Potato starch	94a170123	1
Caelo	Potato starch	17327201	3
Klenk	Potato starch	94A170123	1

- 78 729 spectra from 565 *Apo-Ident* customers from a total of 26 055 batches from a further 690 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Starch* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Starch* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	560	0	73 936
Type B	0	500	0	126 372
Type C	0	197	3	78 725

The substance/substance group *Starch* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.9286 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.8000 %)
Type C	100.0000 % (> 99.8820 %)	98.5000 % (> 97.0000 %)

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
21973	22450	3.27	27.00
22246	24361	7.65	21.77
22585	24361	2.97	18.21
22642	22642	0.00	13.88
20790	23220	4.54	15.94
23220	23220	0.00	13.51
21827	24361	5.70	19.77
24361	24361	0.00	22.43
21447	21447	0.00	19.82
20996	20996	0.00	48.41
21965	22449	4.59	48.10
22449	22449	0.00	42.31
23923	22449	5.73	47.15
22450	22450	0.00	21.17

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Stearic acid 50**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20869-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Stearic acid 50; Acidum stearicum

Special notes

When selecting the *Stearic acid 50* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Stearic acid 50*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Stearic acid 50	12241910	20869	40	AR-15-FG-007284-01
Caelo	Stearic acid 50	14359310	21928	40	AR-16-FG-004044-01
Caelo	Stearic acid 50	14359314	22274	40	20150126

Validation samples

A total of 280 317 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 *Stearic acid 50*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 [†].

- 260 spectra of 7 reference samples from the substance/substance group *Stearic acid 50*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Stearic acid 50	14359310	21793	60
Caelo	Stearic acid 50	14359310	21928 [†]	20
Caelo	Stearic acid 50	14359314	22274 [†]	20
Caelo	Stearic acid 50	163469	23032	40
Caelo	Stearic acid 50	170810	23294	40
Caelo	Stearic acid 50	170810	23667	40
Caelo	Stearic acid 50	180809	24036	40

- 126 632 spectra from a total of 2784 batches from further 781 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 15 *Apo-Ident* customers from 15 batches from the substance/substance group *Stearic acid 50*.

[†]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	Stearic acid 50	11308505	1
Caelo	Stearic acid 50	11103706	1
Caelo	Stearic acid 50	11308514	1
Caesar&Loretz GmbH/Anzag	Stearic acid 50	11308505	1
Caelo	Stearic acid 50	12241911	2
Caelo	Stearic acid 50	12241915	2
Caelo	Stearic acid 50	12241914	1
Phoenix	Stearic acid 50	12241915	1
Phönix	Stearic acid 50	1224915	1
Caelo	Stearic acid 50	12241930	3
Caelo	Stearic acid 50	14359314	2
Caesar & Loretz	Stearic acid 50	14359310	1
Caelo	Stearic acid 50	16096301	1
Caelo	Stearic acid 50	16096311	1
Kehr	Stearic acid 50	16346902	1
Caelo	Stearic acid 50	1609611	1
Caelo	Stearic acid 50	1617081006	1

- 78 907 spectra from 565 *Apo-Ident* customers from a total of 26 122 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Stearic acid 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 *Stearic acid 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	120	0	74 376
Type B	0	260	0	126 632
Type C	0	21	1	78 907

The substance/substance group *Stearic acid 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 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.8817 %)	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
20869	20869	0.00	69.68
21928	21928	0.00	74.13
22274	21928	4.65	66.78

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sucrose**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20372-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sucrose; Saccharum

Special notes

When selecting the *Sucrose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Sucrose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sucrose	13352909	21484	40	1410501
Caelo	Sucrose	14340003	21736	40	20141114
Caelo	Sucrose	163286	23057	40	20161219*

Validation samples

A total of 280 317 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 *Sucrose*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 [†].

- 460 spectra of 12 reference samples from the substance/substance group *Sucrose*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sucrose	12146801	20909	40
Caelo	Sucrose	14340003	21736 [†]	20
Caelo	Sucrose	161999	22615	40
Caelo	Sucrose	162060	22643	40
Caelo	Sucrose	163081	23058	40
Caelo	Sucrose	171066	23297	40
Caelo	Sucrose	172133	23666	40
Caelo	Sucrose	173247	23833	40
Caelo	Sucrose	181582	24217	40
Caelo	Sucrose	181546	24237	40
Caelo	Sucrose	182574	24353	40
Caelo	Sucrose	182818	24359	40

- 126 432 spectra from a total of 2777 batches from further 781 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.

- 332 spectra from 136 *Apo-Ident* customers from 142 batches from the substance/substance group *Sucrose*.

Supplier	Substance	Batch	Spectra
Fagron	Sucrose	11/16-N01	1
Werner	Sucrose	1901208731	2
Fagron	Sucrose	11/20-N05	1
Fagron	Sucrose	11L09-N16	2
Fagron	Sucrose	5071201	1
Soldan	Sucrose	232027	1
Fagron	Sucrose	12G26-N01	2
Fagron	Sucrose	11I16-N01	1
Spagyra	Sucrose	12103020975	1
Caelo	Sucrose	11246313	2
Fagron	Sucrose	11E19-N04	1
Spagyra	Sucrose	12082320717	1
Caelo	Sucrose	12241804	2
Caelo	Sucrose	12241801	1
Fagron	Sucrose	5112I-02207	1
Fagron	Sucrose	11/16-N01	1
Caelo	Sucrose	12241808	5
Caelo	Sucrose	12241803	2
Fagron	Sucrose	12-E03-M01	1
Spagyra	Sucrose	13040921431	1
Spagyra	Sucrose	13040921430	1
Spagyra	Sucrose	13040921424	1
Spagyra	Sucrose	13012920302	1
Spagyra	Sucrose	13020620240	1
Spagyra	Sucrose	13030621373	1
Spagyra	Sucrose	13040921427	1
Spagyra	Sucrose	13041920154	1
Caelo	Sucrose	11246306	1
Staufen-Pharma	Sucrose	161112	2
Spagyra	Sucrose	13041920152	1
Caelo	Sucrose	12241817	2
Haushalt	Sucrose	123456	1
Spagyra	Sucrose	13051520941	1
Spagyra	Sucrose	13051520939	1
Pfeifer/Langen	Sucrose	L03144N	1
Fagron	Sucrose	13A07-N03	1
Spagyra	Sucrose	13061020525	1
Spagyra	Sucrose	13061020526	1
Spagyra	Sucrose	13061020529	1
Spagyra	Sucrose	13061020524	1
Spagyra	Sucrose	13061020528	1
Spagyra	Sucrose	13050621773	2
Spagyra	Sucrose	13061220385	1
Spagyra	Sucrose	13070420937	1
Spagyra	Sucrose	13070420936	1
Spagyra	Sucrose	13070420938	1
Spagyra	Sucrose	13072620834	1
Caelo	Sucrose	13031405	3
Fagron	Sucrose	12E29-N04	1
Caelo	Sucrose	28081308	1
Caelo	Sucrose	12107805	1
Caelo	Sucrose	13031410	2

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Supplier	Substance	Batch	Spectra
Caelo	Sucrose	13063907	1
Fagron	Sucrose	13D29-N08	1
Caelo	Sucrose	13031406	2
Fagron	Sucrose	13G04-N01	1
Fagron	Sucrose	1011208731	2
Caelo	Sucrose	13031414	1
Fagron	Sucrose	13G03-N16	1
Penny Markt	Sucrose	L120325600	2
Caelo	Sucrose	13031417	2
Fagron	Sucrose	13I30-N05	1
Caelo	Sucrose	130031417	1
Caelo	Sucrose	20011401	1
Caelo	Sucrose	13352902	12
Caelo	Sucrose	13352901	2
Caelo	Sucrose	13031409	1
Caelo	Sucrose	12280309	1
Caelo	Sucrose		1
pharm-a-speres	Sucrose	8731003	1
Soldan	Sucrose	243983	1
Soldan	Sucrose		1
Caelo	Sucrose	13352909	4
Caelo	Sucrose	13352905	1
Penny Markt	Sucrose	L120404100	3
Fagron	Sucrose	2102308731	1
	Sucrose	13352908	1
Caelo	Sucrose	13352908	1
Caelo	Sucrose	13352911	1
Fagron	Sucrose	18082014D	1
Caelo	Sucrose	13352920	5
Noweda	Sucrose	13352920	2
Caelo	Sucrose	13352916	3
Caelo	Sucrose	14197302	3
Caelo	Sucrose	1352920	1
Caelo	Sucrose	14197313	1
Caelo	Sucrose	14197301	4
Sanacorp	Sucrose	14340005	1
Kaufland	Sucrose	L24475	1
Kaufland	Sucrose	L24494	2
Caelo	Sucrose	14340003	3
Sanacorp	Sucrose	AKD5	1
Caelo	Sucrose	20031515	1
Caelo	Sucrose	14340009	4
Caelo	Sucrose	14340004	3
Caelo	Sucrose	15028801	10
Caelo	Sucrose	14340006	1
Caelo	Sucrose	14340008	1
Caelo	Sucrose	28041504	1
Caelo	Sucrose	1430009	1
Caelo	Sucrose	24061502	1
Penny	Sucrose	L12513800	3
Caelo	Sucrose	29081502	1
Caelo	Sucrose	15028802	5
Caelo	Sucrose	15182804	16
Caelo	Sucrose	14340005	1
Caelo	Sucrose	15182805	1
Penny Markt	Sucrose	201L113530100	3
Caelo	Sucrose	15446007	1
Jenne	Sucrose	15182804	1
AHD	Sucrose	15182805	1
Caelo	Sucrose	15446002	6

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Supplier	Substance	Batch	Spectra
Caeolo/Gehe	Sucrose	15446002	1
Caelo	Sucrose	15446003	3
Phönix	Sucrose	15446002	1
Penny Markt	Sucrose	L120612100	3
Caelo	Sucrose	154460	1
Fagron	Sucrose	15446002	1
Caelo	Sucrose	81172478	2
Caelo	Sucrose	16049907	12
Caelo	Sucrose	15156008	1
Euro OTC	Sucrose	12345	2
Pharmachem	Sucrose	7878	1
Penny Markt	Sucrose	L120628000	3
Audor Pharma	Sucrose	16206102	1
Caelo	Sucrose	160499	1
Caelo	Sucrose	162061	1
Caelo	Sucrose	16049902	2
Caelo	Sucrose	16206102	9
Bombastus	Sucrose	15156008	1
Caelo	Sucrose	16206103	2
Caelo	Sucrose	16051301	1
Caelo	Sucrose	16328603	6
Caelo	Sucrose	16051305	1
Caelo	Sucrose	16328605	10
Caelo	Sucrose	16328606	2
phönix	Sucrose	16351701	1
Caelo	Sucrose	1649902	1
Kehr	Sucrose	16328606	1
Euro OTC	Sucrose	16328605	1
Caelo	Sucrose	16328607	5
Caelo	Sucrose	13111706	1
Noweda	Sucrose	16328607	1
Caelo	Sucrose	17106603	15
Caelo	Sucrose	17106604	6
Caelo	Sucrose	17042103	1
Gehe	Sucrose	16328607	1
Caelo	Sucrose	17106601	1
Caelo	Sucrose	17354506	5
Caelo	Sucrose	18024405	6
Caelo	Sucrose	18024407	2
Caelo	Sucrose	17247203	1
Caelo	Sucrose	18154603	5
Caelo	Sucrose	1802445	1
Caelo	Sucrose	27111802	1
Caelo	Sucrose	18257402	2

- 78 597 spectra from 565 *Apo-Ident* customers from a total of 25 999 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sucrose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sucrose* and it was evaluated how

many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	420	40	126 432
Type C	0	278	54	78 597

The substance/substance group *Sucrose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	91.3043 % (> 90.6522 %)
Type C	100.0000 % (> 99.8817 %)	83.7349 % (> 82.8313 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21484	21484	0.00	46.74
21736	21484	0.77	46.46
23057	23057	0.00	46.19

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sulfacetamide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20695-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sulfacetamide; Sulfacetamidum

Special notes

When selecting the *Sulfacetamide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Sulfacetamide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfacetamide	11085910	20695	40	1402651
Euro OTC	Sulfacetamide	1312012-01	21633	40	20140117
Euro OTC	Sulfacetamide	1509018	21902	40	20150929*
Caelo	Sulfacetamide	15445901	23251	40	20160126

Validation samples

A total of 280 317 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 *Sulfacetamide*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Sulfacetamide*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sulfacetamide	1312012-01	21633 [†]	20
Euro OTC	Sulfacetamide	1509018	21902 [†]	20
Euro OTC	Sulfacetamide	1702006	23157	40
Caelo	Sulfacetamide	15445901	23456	40
Euro OTC	Sulfacetamide	1808035	24193	40

- 126 732 spectra from a total of 2784 batches from further 781 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*.

- 50 spectra from 21 *Apo-Ident* customers from 21 batches from the substance/substance group *Sulfacetamide*.

Supplier	Substance	Batch	Spectra
Gehe	Sulfacetamide	1112032-01	4
Caelo	Sulfacetamide	10145811	1
Caelo	Sulfacetamide	11085909	1
Gehe	Sulfacetamide	11085904	1
Euro OTC	Sulfacetamide	1112032-01	3
Phönix	Sulfacetamide	11085910	1
Caelo	Sulfacetamide	11085912	3
Caelo	Sulfacetamide	11095912	1
Caelo	Sulfacetamide	11085911	3
Euro OTC	Sulfacetamide	1112032-02	4
Caelo	Sulfacetamide	10145802	1
Caelo	Sulfacetamide	11085913	1
AHC 12.08.13 EK9,31	Sulfacetamide	11085912	1
Caelo	Sulfacetamide	11085914	2
Phönix Gotha	Sulfacetamide	11085911	1
Euro OTC	Sulfacetamide	1312012-01	4
Gehe	Sulfacetamide	1312012-01	2
Industrias GmbH / Ph	Sulfacetamide	64518	1
Euro OTC	Sulfacetamide	1312012-02	2
Gehe	Sulfacetamide	1312012-02	1
Phönix Gotha	Sulfacetamide	1312012-02	1
Euro OTC	Sulfacetamide	1509018-01	4
Gehe	Sulfacetamide	1505025-01	1
Euro OTC	Sulfacetamide	1509018-02	2
Caelo	Sulfacetamide	1509018-02	1
Euro OTC	Sulfacetamide	1702006-01	1
Caelo	Sulfacetamide	15445901	1
Euro OTC	Sulfacetamide	1702006-02	1

- 78 879 spectra from 565 *Apo-Ident* customers from a total of 26 116 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sulfacetamide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfacetamide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	160	0	126 732
Type C	0	45	5	78 879

The substance/substance group *Sulfacetamide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	90.0000 % (> 84.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20695	20695	0.00	47.77
21633	21902	6.28	50.54
21902	21902	0.00	46.52
23251	20695	8.50	54.84

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sulfadiazine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20753-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sulfadiazine; Sulfadiazinum

Special notes

When selecting the *Sulfadiazine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Sulfadiazine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfadiazine	12164101	20753	40	1402053
Caelo	Sulfadiazine	13150011	21744	40	20130708
Caelo	Sulfadiazine	17056602	23447	40	20170330

Validation samples

A total of 280 317 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 *Sulfadiazine*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Sulfadiazine*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfadiazine	13150011	21744 [†]	20
Caelo	Sulfadiazine	170566	23319	40
Caelo	Sulfadiazine	17056602	23374	40
Caelo	Sulfadiazine	172222	23630	30

- 126 762 spectra from a total of 2785 batches from further 781 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 3 batches from the substance/substance group *Sulfadiazine*.

Supplier	Substance	Batch	Spectra
Caelo	Sulfadiazine	11194204	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	Sulfadiazine	13150004	1
Caelo	Sulfadiazine	17358910	3

- 78 924 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sulfadiazine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfadiazine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	130	0	126 762
Type C	0	5	0	78 924

The substance/substance group *Sulfadiazine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.8819 %)	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
20753	20753	0.00	90.28
21744	20753	7.96	89.68
23447	20753	6.33	88.53

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Sulfogaiacol hydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20327-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sulfogaiacol hydrate; Sulfogaiacolum hydricum

Special notes

When selecting the *Sulfogaiacol hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Sulfogaiacol hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfogaiacol hyd...	13405805	21696	30	20140108
Gatt-Koller	Sulfogaiacol hyd...	1156/04152115	21843	40	20150410
Gatt-Koller	Sulfogaiacol hyd...	4543/01170317	23113	40	AR-17-FG-012520-01

Validation samples

A total of 280 317 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 *Sulfogaiacol hydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 386 spectra from a total of 1620 batches from further 372 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 [†].

- 115 spectra of 4 reference samples from the substance/substance group *Sulfogaiacol hydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfogaiacol hydrate	13405805	21696 [†]	15
Gatt-Koller	Sulfogaiacol hydrate	1156/04152115	21843 [†]	20
Caelo	Sulfogaiacol hydrate	170919	23300	40
Caelo	Sulfogaiacol hydrate	170919	23306	40

- 126 777 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 4 *Apo-Ident* customers from 1 batches from the substance/substance group *Sulfogaiacol hydrate*.

Supplier	Substance	Batch	Spectra
Caelo	Sulfogaiacol hydrate	15343912	12

[†]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*.

- 78 917 spectra from 565 *Apo-Ident* customers from a total of 26 136 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sulfogaiacol hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfogaiacol hydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 386
Type B	0	115	0	126 777
Type C	0	3	9	78 917

The substance/substance group *Sulfogaiacol hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 94.5455 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.7826 %)
Type C	100.0000 % (> 99.8818 %)	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
21696	23113	8.10	74.36
21843	23113	7.87	75.61
23113	23113	0.00	71.33

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **SyrSpend[®] SF alka / pH4**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 22496-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

SyrSpend[®] SF alka / pH4; SyrSpend[®] SF Alka; SyrSpend[®] SF pH4

Special notes

When selecting the *SyrSpend[®] SF alka / pH4* substance/substance group, the following information is displayed to the user:

- Hinweis zur Identifizierung von SyrSpend[®] SF Alka: Bitte Probe vor der Messung schütteln, um eine gleichmäßige Partikelverteilung zu gewährleisten.

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *SyrSpend[®] SF alka / pH4*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	SyrSpend [®] SF pH4	15A26-B04-311720	22496	40	1608352
Fagron	SyrSpend [®] SF pH4	15A26-B04-305667	22719	40	1701055
Fagron	SyrSpend [®] SF Alka	17D11-B04-332593	23448	40	20170505
Fagron	SyrSpend [®] SF Alka	17F14-B02-335945	23750	20	1804106
Fagron	SyrSpend [®] SF Alka	18B21-B08-347192	24112	40	1809264
Fagron	SyrSpend [®] SF Alka	18C13-B11-350851	24290	40	20180502

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 6 reference samples from the substance/substance group *SyrSpend[®] SF alka / pH4*. These samples are listed above in the [calibration samples](#) section.
- 74276 spectra from a total of 1617 batches from further 371 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 *SyrSpend[®] SF alka / pH4*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	SyrSpend [®] SF Alka	15H11-B04-311722	22494	40
Fagron	SyrSpend [®] SF Alka	15H11-B04-311722	22495	40
Fagron	SyrSpend [®] SF pH4	15A26-B04-311720	22497	40
Fagron	SyrSpend [®] SF Alka	15H11-B04-311722	22718	40
Fagron	SyrSpend [®] SF Alka	17D11-B04-332593	23449	40
Fagron	SyrSpend [®] SF pH4	15H13-B03-314611	23450	40
Fagron	SyrSpend [®] SF pH4	15H13-B03-314611	23451	40
Fagron	SyrSpend [®] SF pH4	16J10-B03-330757	23749	40
Fagron	SyrSpend [®] SF Alka	17F14-B02-335945	23750 [†]	20
Fagron	SyrSpend [®] SF Alka	15H11-B04-311722	23768	40

- 126512 spectra from a total of 2783 batches from further 780 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

[†]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.

- 20 spectra from 15 *Apo-Ident* customers from 15 batches from the substance/substance group *SyrSpend[®] SF alka / pH4*.

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend [®] SF Alka	16B03-B07-525234	1
Fagron	SyrSpend [®] SF Alka	17D11-B04-332593	1
Fagron	SyrSpend [®] SF Alka	15K03-B01-525173	1
Fagron	SyrSpend [®] SF Alka	17D11-B04	2
Fagron	SyrSpend [®] SF Alka	17D11-bo4-332593	1
Fagron	SyrSpend [®] SF Alka	18A26-B05-346410	1
Fagron	SyrSpend [®] SF Alka	17F14-B02-335945	1
Phönix/Fagon	SyrSpend [®] SF Alka	17D11-B04-332593	1
Fagron	SyrSpend [®] SF Alka	18A26-Bo5-346410	1
Fagron	SyrSpend [®] SF Alka	17D11-804-332593	1
Caelo	SyrSpend [®] SF Alka	18C13-B11-350851	1
Fagron	SyrSpend [®] SF Alka	18C13-B11-350851	1
Fagron	SyrSpend [®] SF Alka	18H01-B12-353473	1
Fagron	SyrSpend [®] SF pH4	16J10-B03-330757	3
Fagron	SyrSpend [®] SF pH4	16/10-B03	1
Fagron	SyrSpend [®] SF pH4	16J10B03	1
Fagron	SyrSpend [®] SF pH4	18A22-B05-346147	1

- 78 909 spectra from 565 *Apo-Ident* customers from a total of 26 122 batches from a further 692 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *SyrSpend[®] SF alka / pH4* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *SyrSpend[®] SF alka / pH4* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	220	0	74 276
Type B	0	380	0	126 511
Type C	0	20	0	78 909

The substance/substance group *SyrSpend[®] SF alka / pH4* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 70.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22496	22496	0.00	21.92
22719	22719	0.00	13.95
23448	24112	6.31	23.93
23750	23750	0.00	22.81
24112	24112	0.00	25.41
24290	24112	2.68	25.55

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tannin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20018-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tannin; Tanninum

Special notes

When selecting the *Tannin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tannin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tannin	12336016	21608	40	20121127
Fagron	Tannin	13H30-B03-287645	21653	40	1711482
Fagron	Tannin	16D08-B04-328410	23211	40	AR-17-FG-015963-01
Caelo	Tannin	172092	23631	40	20170829*

Validation samples

A total of 280 317 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 *Tannin*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Tannin*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tannin	12336016	21608 [†]	20
Fagron	Tannin	13H30-B03-287645	21653 [†]	20
Caelo	Tannin	16074504	23205	40
Fagron	Tannin	16D08-B04-328410	23501	40

- 126 772 spectra from a total of 2785 batches from further 781 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*.

- 252 spectra from 154 *Apo-Ident* customers from 95 batches from the substance/substance group *Tannin*.

Supplier	Substance	Batch	Spectra
Caelo	Tannin	10019007	1
Caelo	Tannin	11302307	5
Caelo	Tannin	10315107	2
Caelo	Tannin	12171101	4
Caelo	Tannin	10315110	2
Caelo	Tannin	9128608	1
Fagron	Tannin	11C09-N05	1
Caesar/Lorenz	Tannin	11302307	1
Fagron	Tannin	12E21-N04	4
Phönix	Tannin	10315110	1
Caelo	Tannin	12171103	2
Caelo	Tannin	12171106	7
Gehe	Tannin	12171106	1
Fagron	Tannin	13B28-N08	1
Fagron	Tannin	12A27-N01	1
Fagron	Tannin	12H14-N05	5
Caelo	Tannin	12336001	11
Sanacorp	Tannin	12171102	1
A.H.D.	Tannin	13E27-N08	1
Caelo	Tannin	12A27-N01	1
Caelo	Tannin	21101305	1
Hirsch	Tannin	1811209	1
Fagron	Tannin	12H14N05	1
Nachprüfung	Tannin	5210A-01052	1
Caelo	Tannin	4413I1052	1
Alliance Healthcare	Tannin	12336001	1
Caelo	Tannin	12336009	10
Caelo	Tannin	12336001	1
Phönix	Tannin	10313107Retest	1
Caelo	Tannin	12336007	2
Caelo	Tannin	12336005	2
Caelo	Tannin	2211Q-01052	1
Caelo	Tannin	12336013	5
Fagron	Tannin	13E27-N08	1
Sanacorp	Tannin	12336011	1
Caelo	Tannin	12336014	5
Gehe	Tannin	12H14-N05	1
Synopharm/Anzag	Tannin	3411I-01052	1
Fagron	Tannin	13H30-B03-287645	2
Caelo	Tannin	13031401	1
Fagron	Tannin	13H30-B03287645	1
Phoenix	Tannin	12336013	1
Sanacorp	Tannin		1
Gehe	Tannin	12336016	2
Caelo	Tannin	12336016	7
Sanacorp	Tannin	12336014	1
Gatt-Koller / Phoenix	Tannin	333508134613	2
Gatt-Koller / Phoenix	Tannin	3335/08134613	1
Fagron	Tannin	14A07-B01-293468	5
Caelo	Tannin	14031901	2
Fagron	Tannin	2212M-01052	1
Caelo	Tannin	14031903	4
Caelo	Tannin	14031905	3
Caelo	Tannin	12336011	1
Caelo	Tannin	14031912	3
Fagron	Tannin	160300146	2
Sanacorp	Tannin	14031912	1

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Supplier	Substance	Batch	Spectra
Caelo	Tannin	28011502	1
Caelo	Tannin	14031915	2
phönix	Tannin	15/AKD65	1
Fagron	Tannin	160300126	1
Fagron	Tannin	14E07-B03-298480	2
Fagron	Tannin	14J06-B04-0858	1
Caelo	Tannin	14031913	2
Caelo	Tannin	14031918	3
Caelo	Tannin	14031919	5
Fagron	Tannin	14J06-B04	1
Caelo	Tannin	14031920	1
Caelo	Tannin	15091504	4
Caelo	Tannin	15243801	8
Fagron	Tannin	14J06-B04-299398	1
Caelo	Tannin	15243802	3
Caelo	Tannin	1524308	1
Fagron	Tannin	14J06B04299398	1
Caelo	Tannin	15091506	1
Caleo/Phoenix	Tannin	14K17-B08-306993	1
Caelo	Tannin	15091503	1
Fagron	Tannin	14e07-b03-298480	1
Fagron	Tannin	160300029	1
Caelo	Tannin	15091509	13
Ebert u. Jacobi 16.0...	Tannin	15091509	1
Fagron	Tannin	1014A-01052	1
Caelo	Tannin	15091512	1
Caelo	Tannin	15091511	2
Caelo	Tannin	15091515	7
Fagron	Tannin	15F23-B01-322984	2
ALH	Tannin	15091515	1
ALH	Tannin	14031919	1
Fagron	Tannin	15F23-B01-326357	1
Caelo	Tannin	15F23-B01-326357	1
Fagron	Tannin	15F23-B01	1
Caelo	Tannin	16074504	10
Euro OTC	Tannin	16074501	1
Frago/Gehe	Tannin	15F23-B01	1
Fagron	Tannin	15F23B01326357	1
phönix	Tannin	14E07-B03-293744	1
Gehe	Tannin	16074504	1
Caelo	Tannin	16074505	1
Caelo	Tannin	16D08-B04-328410	1
Caelo	Tannin	16074509	6
Fagron	Tannin	160300178B	2
Fagron	Tannin	16D08-b04	1
Fagron	Tannin	16D08-B04-334834	2
Noweda	Tannin	16074509	1
Caelo	Tannin	16074509/171027T	1
Fagron	Tannin	16D08-B04-328410	1
Caelo	Tannin	16074516	3
Caelo	Tannin		1
Caelo	Tannin	16074518	4
Caelo	Tannin	16074517	1
Sanacorp WE: 26.01.15 E...	Tannin	14031912	1
Caelo	Tannin	18017701	1
Caelo	Tannin	17343503	1
Caelo	Tannin	17343504	1
Caelo	Tannin	17343502	1
Caelo	Tannin	17343505	1

- 78 677 spectra from 565 *Apo-Ident* customers from a total of 26 043 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tannin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tannin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	120	0	126 772
Type C	0	248	4	78 677

The substance/substance group *Tannin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	98.4127 % (> 97.2222 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21608	21653	10.96	47.45
21653	21653	0.00	47.92
23211	23211	0.00	48.27
23631	23631	0.00	47.23

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tartaric acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20014-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tartaric acid; Acidum tartaricum

Special notes

When selecting the *Tartaric acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tartaric acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tartaric acid	15130201	22383	40	20150416
Caelo	Tartaric acid	15164001	22384	40	1704461
Fagron	Tartaric acid	13I25-B01-294093	22391	40	1711509
Fagron	Tartaric acid	14G07-B02-308554	22501	40	20140827
Caelo	Tartaric acid	161468	22613	40	20160607*

Validation samples

A total of 280317 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 *Tartaric acid*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1618 batches from further 372 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 *Tartaric acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tartaric acid	13217803	21457	60
Caelo	Tartaric acid	15130201	22383 [†]	20
Caelo	Tartaric acid	15164001	22384 [†]	20
Fagron	Tartaric acid	13I25-B01-294093	22391 [†]	20
Fagron	Tartaric acid	14G07-B02-322976	23527	40
Caelo	Tartaric acid	181212	24015	40

- 126692 spectra from a total of 2783 batches from further 781 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*.

- 191 spectra from 100 *Apo-Ident* customers from 112 batches from the substance/substance group *Tartaric acid*.

Supplier	Substance	Batch	Spectra
apomix	Tartaric acid		1
Spangropharm	Tartaric acid	10073111	1
apomix	Tartaric acid	1111	1
Fagron	Tartaric acid	1106211053	1
Fagron	Tartaric acid	11E24-N06	1
Phönix	Tartaric acid	11e24-n06	1
Caelo	Tartaric acid	10180708	2
Caelo	Tartaric acid	12044101	2
Caelo	Tartaric acid	11k10-n07	1
Caelo	Tartaric acid	1169406	1
Caelo	Tartaric acid	12044103	4
Caelo	Tartaric acid	11169406	2
Fagron	Tartaric acid	20151112-2	1
Caelo	Tartaric acid	10180713	2
Fagron	Tartaric acid	xxxxxxx	1
Caelo	Tartaric acid		1
Caelo	Tartaric acid	10199713	1
Phoenix	Tartaric acid	12044115	1
Noweda/ Fischar	Tartaric acid	702061	1
Gehe	Tartaric acid	7284696	1
Fagron	Tartaric acid	12F18-No2	1
Fagron	Tartaric acid	12F18-N02	1
Caelo	Tartaric acid	12044102	3
Caelo	Tartaric acid	1204102	1
Fagron	Tartaric acid	12K16-N02	1
Fagron	Tartaric acid	2513M01053	1
Caelo	Tartaric acid	12286903	2
Fagron	Tartaric acid	12131	2
Caelo	Tartaric acid	10180714	1
Caesar & Loretz/ Noweda	Tartaric acid	12044103	1
Fagron	Tartaric acid	13B15-N01	7
Caelo	Tartaric acid	12044119	3
Fagron	Tartaric acid	12H02-N07	3
Caelo	Tartaric acid	4110N-01053	1
Phoenix	Tartaric acid	12Ho2-N07	1
Fagron	Tartaric acid	13B15N01	1
Caelo	Tartaric acid	12H02-n07	1
Caelo	Tartaric acid	12286906	3
Fagron	Tartaric acid	11E24-N060752/764	1
Caelo	Tartaric acid	9494239	1
canea, anzag	Tartaric acid	12286906	1
Caelo	Tartaric acid	12240402	1
Caelo	Tartaric acid	12240415	1
Fragon/Sanacorp	Tartaric acid	13G03-N14	2
Caelo	Tartaric acid	13B15-N01	2
Gehe	Tartaric acid	703061	1
Phönix	Tartaric acid	12286904	1
Caelo	Tartaric acid	12240413	1
Phoenix	Tartaric acid	13116308	1
Caelo	Tartaric acid	13116307	1
Caelo	Tartaric acid	12286911	1
Caelo	Tartaric acid	13116308	2
Caelo	Tartaric acid	13116306	1
Phoenix	Tartaric acid	12K29B01	1
Fagron	Tartaric acid	13125-B01-285488	1

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Supplier	Substance	Batch	Spectra
Fagron	Tartaric acid	13/25-B01-285488	2
Caelo	Tartaric acid	12286904	1
Fagron	Tartaric acid	2414E1053	1
Caelo	Tartaric acid	12286924	1
GEHE 14.04.2014	Tartaric acid	13G03-N14	2
GEHE 14.04.2014	Tartaric acid	12H02-N07	1
Fagron	Tartaric acid	13I25-B01-285488	2
Gehe	Tartaric acid	1325-B01-285487	1
Gatt-Koller / Phoenix	Tartaric acid	3334/08131514	1
Fagron	Tartaric acid	12K29-B01-285247	1
schubert / Phoenix	Tartaric acid	1014PLV-755	1
Caelo	Tartaric acid	17091402	1
Caelo	Tartaric acid	13217807	1
Caelo	Tartaric acid	12286934	1
Caelo	Tartaric acid	12286932	1
Caelo	Tartaric acid	14054521	1
Caelo	Tartaric acid	13217806	2
Fagron	Tartaric acid	13I25-B01-285487	1
Fagron	Tartaric acid	13I25-B01-294094	3
Fagron	Tartaric acid	13/25-B01-285487	1
Fagron	Tartaric acid	13I25-B01-294093	1
Caelo	Tartaric acid	12286939	1
Caelo	Tartaric acid	14186213	4
Fischar/Phönix	Tartaric acid	704021	1
Fagron	Tartaric acid	13I25-B01-294095	1
Fagron	Tartaric acid	1325-B01-294093	1
Phönix Gotha	Tartaric acid	704021	1
Caelo	Tartaric acid	15045304	1
Fagron	Tartaric acid	15045303	1
Fischar	Tartaric acid	704061	2
Caelo	Tartaric acid	15164001	3
Caelo	Tartaric acid	15130201	6
Fagron	Tartaric acid	14186212	1
Caelo	Tartaric acid	15045303	1
Caelo	Tartaric acid	15130205	2
Caelo	Tartaric acid	15164002	3
Caelo	Tartaric acid	151302	1
Otto Fischar	Tartaric acid	705061	2
Beiersdorf AG	Tartaric acid	11G19-N08	1
Fagron	Tartaric acid	14G07-B02-308554	1
Caelo	Tartaric acid	13I25-B01-294093	1
Caelo	Tartaric acid	15164008	2
Caelo	Tartaric acid	15164010	1
Caelo	Tartaric acid	15130206	1
Fischar	Tartaric acid	705061	1
Caelo	Tartaric acid	15349101	1
Caelo	Tartaric acid	14G07-B02-308555	1
Caelo	Tartaric acid	15349109	4
Euro OTC	Tartaric acid	702265	1
Caelo	Tartaric acid	15349105	4
Otto Fischer GmbH	Tartaric acid	705061	1
Gehe/Fischer	Tartaric acid	706061	1
Caelo	Tartaric acid	9041703	1
Fagron	Tartaric acid	14519	1
Gehe	Tartaric acid	16146806	1
Caelo	Tartaric acid	15349106	2
Fagron	Tartaric acid	14G07-B02	1
Caelo	Tartaric acid	16260403	2
Caelo	Tartaric acid	15349102	1
Fagron	Tartaric acid	1325-B01-294094	1

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Supplier	Substance	Batch	Spectra
Caelo	Tartaric acid	15349110	2
Caelo	Tartaric acid	16260404	4
Gehe/Henry Lamotte	Tartaric acid	17/12	1
Fagron	Tartaric acid	13G03-N14	1
Caelo	Tartaric acid	16260406	3
Caelo	Tartaric acid	16260405	1
Caelo	Tartaric acid	8051809	1
Sanacorp WE: 19.0518 EK...	Tartaric acid	16260406	1
Caelo	Tartaric acid	16146806	1
Fagron	Tartaric acid	14G07-802	1
Euro OTC	Tartaric acid	1604046-02	1
Fischar/Gehe	Tartaric acid	705061	1
Caelo	Tartaric acid	17347104	1
Sanacorp	Tartaric acid	17347104	1

- 78 738 spectra from 565 *Apo-Ident* customers from a total of 26 026 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tartaric 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 *Tartaric 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	200	0	74 296
Type B	0	200	0	126 692
Type C	0	183	8	78 738

The substance/substance group *Tartaric 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 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8817 %)	95.8115 % (> 94.2408 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22383	22613	3.90	35.05
22384	22384	0.00	35.90
22391	22391	0.00	35.41
22501	22391	2.66	35.66
22613	22613	0.00	35.28

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Taurine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20403-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Taurine; Taurinum

Special notes

When selecting the *Taurine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Taurine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Taurine	1306024-01	21108	40	20130822
Euro OTC	Taurine	1504032-01	21893	40	20150430
Euro OTC	Taurine	1504032-01	21992	40	9167
Euro OTC	Taurine	1602011	22370	40	20160218*

Validation samples

A total of 280317 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 *Taurine*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1620 batches from further 372 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 [†].

- 230 spectra of 8 reference samples from the substance/substance group *Taurine*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Taurine	1306024-01	21108 [†]	10
Euro OTC	Taurine	1504032-01	21893 [†]	20
Euro OTC	Taurine	1504032-01	21992 [†]	20
Euro OTC	Taurine	1602011	22370 [†]	20
Euro OTC	Taurine	1607035	22795	40
Euro OTC	Taurine	1704001	23177	40
Euro OTC	Taurine	1711006	23739	40
Euro OTC	Taurine	1810006	24310	40

- 126662 spectra from a total of 2782 batches from further 781 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.

- 5 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Taurine*.

Supplier	Substance	Batch	Spectra
hannes	Taurine	1202125	1
Gall Pharma / Phoenix	Taurine		1
elcompra	Taurine	xp17013244	1
el compra import	Taurine	1609025	1
Euro OTC	Taurine	1704001-01	1

- 78 924 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Taurine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Taurine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	230	0	126 662
Type C	0	5	0	78 924

The substance/substance group *Taurine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.3913 %)
Type C	100.0000 % (> 99.8819 %)	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
21108	22370	3.01	57.68
21893	21992	0.99	63.01
21992	21992	0.00	60.80
22370	22370	0.00	60.33

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Testosterone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20961-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Testosterone; Testosteronum

Special notes

When selecting the *Testosterone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Testosterone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Testosterone	12F13-N02	20729	40	20120628
Euro OTC	Testosterone	1307001-01	20961	40	1402309
Caelo	Testosterone	13406004	21370	50	20131219
Fagron	Testosterone	15E18-B08-307772	21970	40	20150526
Caelo	Testosterone	15244906	21987	40	20150814

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Testosterone	1511005	22232	40	20151119*
Euro OTC	Testosterone	1604049	22561	40	20160510*
Caelo	Testosterone	16311506	23244	40	20161123
Fagron	Testosterone	17J26-B01-342032	23764	40	20171205
Fagron	Testosterone	15E18-B08-307772	21970SI	35	20150526
Caelo	Testosterone	15244906	21987SI	24	20150814
Euro OTC	Testosterone	1511005	22232SI	25	20151119*
Euro OTC	Testosterone	1604049	22561SI	34	20160510*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 488 spectra of 13 reference samples from the substance/substance group *Testosterone*. These samples are listed above in the [calibration samples](#) section.
- 74008 spectra from a total of 1614 batches from further 372 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 [†].

- 1050 spectra of 31 reference samples from the substance/substance group *Testosterone*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Testosterone	13406004	21371	50
Fagron	Testosterone	15E18-B08-307772	21970 [†]	20
Caelo	Testosterone	15244906	21987 [†]	20
Euro OTC	Testosterone	1511005-01	21994	60
Euro OTC	Testosterone	1511005	22232 [†]	20
Euro OTC	Testosterone	1607013	22707	40
Euro OTC	Testosterone	1702017	23146	40
Caelo	Testosterone	171199	23347	40
Caelo	Testosterone	171199	23670	40
Euro OTC	Testosterone	1802015	23948	40
Euro OTC	Testosterone	1805006	24131	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
Euro OTC	Testosterone	1805021	24132	40
Euro OTC	Testosterone	1808033	24201	40
Caelo	Testosterone	181478	24265	40
Euro OTC	Testosterone	1811027	24422	40
Fagron	Testosterone	15E18-B08-307772	21970SI [†]	19
Caelo	Testosterone	15244906	21987SI [†]	14
Euro OTC	Testosterone	1511005-01	21994SI	32
Euro OTC	Testosterone	1511005	22232SI [†]	10
Euro OTC	Testosterone	1607013	22707SI	40
Euro OTC	Testosterone	1702017	23146SI	21
Caelo	Testosterone	16311506	23244SI	30
Caelo	Testosterone	171199	23347SI	28
Caelo	Testosterone	171199	23670SI	30
Fagron	Testosterone	17J26-B01-342032	23764SI	30
Euro OTC	Testosterone	1802015	23948SI	40
Euro OTC	Testosterone	1805006	24131SI	40
Euro OTC	Testosterone	1805021	24132SI	40
Euro OTC	Testosterone	1808033	24201SI	40
Caelo	Testosterone	181478	24265SI	40
Euro OTC	Testosterone	1811027	24422SI	26

- 125 842 spectra from a total of 2773 batches from further 781 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 47 *Apo-Ident* customers from 52 batches from the substance/substance group *Testosterone*.

Supplier	Substance	Batch	Spectra
Fagron	Testosterone	12F13-N02	1
Caelo	Testosterone	APL00034466T	1
Caelo	Testosterone	12176301	1
Euro OTC	Testosterone	3x1106011-03	1
Euro OTC	Testosterone	1106011-03	4
Euro OTC	Testosterone	1106011-01	1
Caelo	Testosterone	12176305	3
Euro OTC	Testosterone	1207005-02	1
Caelo	Testosterone	13134804	1
Fagron	Testosterone	11/07-N12	2
Euro OTC	Testosterone	1307001-01	5
EUro/AHD	Testosterone	1106011-03	1
Caelo	Testosterone	13134806	4
Phoenix Gotha	Testosterone	1106011-03	1
Haihang Industry	Testosterone	20140114-2	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
Haihang Industry	Testosterone	20140114-1	1
Spirig	Testosterone	13406003	1
Caelo	Testosterone	13406004	2
Fagron	Testosterone	13G10-N03	2
Fagron	Testosterone	13I26-N08	1
Euroo/Phoenix	Testosterone	1307001-01	1
Caelo	Testosterone		1
Fagron	Testosterone	13g10n03	1
Fagron	Testosterone	13109b03294149	1
Fagron	Testosterone	13109b03298118	1
Euro OTC	Testosterone	11o6011-03	1
Euro OTC	Testosterone	1404002-01	2
Caelo	Testosterone	14201105	1
NWM CHina	Testosterone	TE150402	1
Caelo	Testosterone	14355605	1
Fagron	Testosterone	13L09-B03-294148	1
Phönix Gotha	Testosterone	1408015-01	1
Euro OTC	Testosterone	140400201	1
Fagron	Testosterone	15E18-B08	1
Euro OTC	Testosterone	1404002-1	1
Caelo	Testosterone	15195802	1
Caelo	Testosterone	15195803	1
Fagron	Testosterone	GTJ151103	1
Euro OTC	Testosterone	1511005-01	3
Caelo	Testosterone	15412202	2
Caelo	Testosterone	15412201	3
Euro OTC	Testosterone	1604049-01	2
Shandong Northwest Manu...	Testosterone	GTJ160510	1
Caelo	Testosterone	1604049-01	1
Euro OTC	Testosterone	1607013-02	1
Fagron	Testosterone	1712-B05	1
Audor Pharma	Testosterone	APZTST16001-M1T	1
Euro OTC	Testosterone	1702017-01	5
Fagron	Testosterone	17A12-B05-331496	1
Audor Pharma	Testosterone	AP5106061T	5
Caelo	Testosterone	AP5106061T	1
Fagron	Testosterone	17J26-B01-342033	2
Noweda	Testosterone	1702017-01	1
Audor Pharma	Testosterone	APZTSTG18003T	8
Caelo	Testosterone	17119902	1
Euro OTC	Testosterone	180506-01	1
Audor Pharma	Testosterone	APZTSTG18004T	2
Euro OTC	Testosterone	1805021-01	1

- 78 832 spectra from 565 *Apo-Ident* customers from a total of 26 086 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Testosterone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Testosterone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	488	0	74 008
Type B	0	1009	41	125 842
Type C	0	93	4	78 832

The substance/substance group *Testosterone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.7705 %)
Type B	100.0000 % (> 99.9901 %)	96.0952 % (> 95.8095 %)
Type C	100.0000 % (> 99.8817 %)	95.8763 % (> 92.7835 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21970	22232	3.93	21.67
21987	22232	3.04	27.49
22232	22232	0.00	26.36
23244	22232	6.36	20.11
23764	20961	5.64	21.25
22561	22561	0.00	40.73
20961	20961	0.00	23.35
20729	20961	12.22	34.70
21370	22232	5.60	23.18

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Testosterone propionate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20880-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Testosterone propionate; Testosteroni propionas

Special notes

When selecting the *Testosterone propionate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Testosterone propionate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Testosterone pro...	12163607	20880	40	AR-15-FG-000623-01
Euro OTC	Testosterone pro...	1109024-02	21644	40	1503607
Euro OTC	Testosterone pro...	1511003	22230	40	20151111*
Euro OTC	Testosterone pro...	1512023	22288	30	20151230*
Caelo	Testosterone pro...	15444709	23170	40	1707612
Euro OTC	Testosterone pro...	1511003	22230SI	28	20151111*
Euro OTC	Testosterone pro...	1512023	22288SI	30	20151230*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 248 spectra of 7 reference samples from the substance/substance group *Testosterone propionate*. These samples are listed above in the [calibration samples](#) section.
- 74248 spectra from a total of 1618 batches from further 372 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 [†].

- 344 spectra of 12 reference samples from the substance/substance group *Testosterone propionate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Testosterone propionate	1109024-02	21644 [†]	20
Euro OTC	Testosterone propionate	1511003	22230 [†]	20
Euro OTC	Testosterone propionate	1512023	22288 [†]	15
Caelo	Testosterone propionate	170963	23334	40
Euro OTC	Testosterone propionate	1710027	23734	40
Euro OTC	Testosterone propionate	1811040	24413	40
Euro OTC	Testosterone propionate	1511003	22230SI [†]	15
Euro OTC	Testosterone propionate	1512023	22288SI [†]	15
Caelo	Testosterone propionate	15444709	23170SI	30
Caelo	Testosterone propionate	170963	23334SI	29
Euro OTC	Testosterone propionate	1710027	23734SI	40
Euro OTC	Testosterone propionate	1811040	24413SI	40

- 126548 spectra from a total of 2782 batches from further 781 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.

- 318 spectra from 167 *Apo-Ident* customers from 132 batches from the substance/substance group *Testosterone propionate*.

Supplier	Substance	Batch	Spectra
Fagron	Testosterone propionate	11C21-N09	1
Fagron	Testosterone propionate	11K18-N04	3
Caelo	Testosterone propionate	106212376	1
Fagron	Testosterone propionate	12E29-N02	1
Fagron	Testosterone propionate	6081201	1
Caelo	Testosterone propionate	1108212376	1
Fagron	Testosterone propionate	12A02-N05	2
Caelo	Testosterone propionate	12060102	2
Caelo	Testosterone propionate	12A02-N05	1
Caelo	Testosterone propionate	612212376	1
Fagron	Testosterone propionate		1
Fagron	Testosterone propionate	20121012-3	1
Fagron	Testosterone propionate	12J10-N08	3
Fagron	Testosterone propionate	12E04-N01	2
Audor Pharma	Testosterone propionate	AP12E04N01TP	2
Fagron	Testosterone propionate	12/10-N08	1
Phönix/Euro	Testosterone propionate	110301002	1
Caelo	Testosterone propionate	12163605	2
Caelo	Testosterone propionate	12J10-N08	2
Caelo	Testosterone propionate	903312376	1
Euro OTC	Testosterone propionate	970116/1	1
Caelo	Testosterone propionate	10235809	1
Fagron	Testosterone propionate	24411M1	1
Fagron	Testosterone propionate	12C01-N01	1
Fagron	Testosterone propionate	13C08-N02	14
Fagron	Testosterone propionate	11/12-N03	1
AHD	Testosterone propionate	AP12E04-N01TP	1
Caelo	Testosterone propionate	2013U-02376	1
Noweda	Testosterone propionate	12163610	1
Audor Pharma	Testosterone propionate	AP12J10-N08TP	2
Phönix	Testosterone propionate	13C08-N02	1
Caelo	Testosterone propionate	12163610	2
Caelo	Testosterone propionate	12163612	6
Fagron	Testosterone propionate	13C08N02	1
Euro OTC	Testosterone propionate	1103010-01	1
Caelo	Testosterone propionate	1263607	1
Fagron	Testosterone propionate	3613M-02376	1
Fagron	Testosterone propionate	32012M1	1
Fagron	Testosterone propionate	12J10N-08	1
Fagron	Testosterone propionate	13F05-N04	15
Fagron	Testosterone propionate	10L03-N16	3
Phönix	Testosterone propionate	12J10-N08	1
Caelo	Testosterone propionate	12163616	4
Andor	Testosterone propionate	1109024-03TP	1
Caelo	Testosterone propionate	12163615	1
Caelo	Testosterone propionate	614E2376	1
Fagron	Testosterone propionate	12163616	2
Fagron	Testosterone propionate	13I03-N02	1

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Supplier	Substance	Batch	Spectra
Audor Pharma	Testosterone propionate	AP1109024-03TP	4
Fagron	Testosterone propionate	13K25-B05-287648	5
Apomix / AHD	Testosterone propionate	40/14	1
Euro OTC	Testosterone propionate	1109024-03	1
Caelo	Testosterone propionate	12163613	1
Fagron	Testosterone propionate	13/03-N02	1
Phoenix	Testosterone propionate	1109024-02	1
Audor Pharma	Testosterone propionate	AP1109024-03	2
Fagron	Testosterone propionate	13K25-B05-291974	2
Fagron	Testosterone propionate	13K25-B05-287647	8
Fagron	Testosterone propionate	36513M1	2
Fagron	Testosterone propionate	14A28-B12-291977	1
apomix	Testosterone propionate	13K25-B05-287648	1
Caelo	Testosterone propionate	12163617	4
Caelo	Testosterone propionate	12163619	2
Caelo	Testosterone propionate	13C08-N02	1
Phönix	Testosterone propionate	12163617	1
Phönix	Testosterone propionate	12163613	1
phoenix	Testosterone propionate	12163615	1
Caelo	Testosterone propionate	12163621	1
Caelo	Testosterone propionate	13K25-B05-291974	1
Fagron	Testosterone propionate	13K25B05287648	1
Phönix	Testosterone propionate	13K25-B05	1
Fagron	Testosterone propionate	14A28-B12-296960	1
Fagron	Testosterone propionate	14D15-B03-296959	4
Euro OTC	Testosterone propionate	1409037-01	2
Fagron	Testosterone propionate	14A28-B12	2
Fagron	Testosterone propionate	13K25-B05	1
Caelo	Testosterone propionate	15003002	8
Caelo	Testosterone propionate	1109024-02	1
Caelo	Testosterone propionate	15003004	2
Caelo	Testosterone propionate	103004	1
Caelo	Testosterone propionate	15003008	2
Gatt-Koller	Testosterone propionate	606213811	1
Fagron	Testosterone propionate	14L31-B02-304722	8
Fagron	Testosterone propionate	14L31-B02	2
Fagron	Testosterone propionate	14A28-B12-296958	2
Fagron	Testosterone propionate	14L31B02304722	1
Caelo	Testosterone propionate	14D15-B03-296959	1
Euro OTC	Testosterone propionate	1103010-02	1
Caelo	Testosterone propionate	14L31-B02-304722	1
Audor Pharma	Testosterone propionate	AP13K25-B05-287643TP	1
Caelo	Testosterone propionate	15169504	1
Anzag	Testosterone propionate	14L31-B02-304722	1
Gatt-Koller	Testosterone propionate	3478/09153915	1
Audor Pharma	Testosterone propionate	AP13K25-B05-287643T	1
Fagron	Testosterone propionate	15D03-B02-310694	1
Euro OTC	Testosterone propionate	1504023-01	1
Symbiotica Speciality	Testosterone propionate	15444702	2
Caelo	Testosterone propionate	15444703	9
Fagron	Testosterone propionate	15K03-B03-315218	6
Fagron	Testosterone propionate	1501-B09-312867	1
Fagron	Testosterone propionate	14L31B02-304721	1
Fagron	Testosterone propionate	14L31-B02-304721	6
Caelo	Testosterone propionate	36814M1	1
Fagron	Testosterone propionate	36814M1	2
Fagron	Testosterone propionate	15K03-B-03-315218	1
Phönix WE:25.04.16 EK:1...	Testosterone propionate	14L31-B02-304722	1
Fagron	Testosterone propionate	11G15-N07	1
Galderma	Testosterone propionate	15K03-B03-315218	1

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Supplier	Substance	Batch	Spectra
Phönix	Testosterone propionate	14L31-B02-304722	1
Caelo	Testosterone propionate	15444702	5
Euro OTC	Testosterone propionate	1511003-01	6
Caelo	Testosterone propionate	36814m1	1
Fagron	Testosterone propionate	15k03-b03	1
Sanacorp	Testosterone propionate	14L31-B02-304721	2
Phönix	Testosterone propionate	15444702	1
Ebert 17.08.16	Testosterone propionate	15444703	1
Fagron	Testosterone propionate	16C24B04320784	1
Fagron	Testosterone propionate	15I01-B09-312867	1
allianz	Testosterone propionate	15444704	1
Fagron	Testosterone propionate	15/01-B09-318371	1
Audor Pharma	Testosterone propionate	APZTSP15003-MTP	7
Fagron	Testosterone propionate	15I01-B09-318371	1
Caelo	Testosterone propionate	15444705	2
AHL	Testosterone propionate	APZTSP15003-MTP	2
Fagron	Testosterone propionate	15/01-B09	1
Fagron	Testosterone propionate	16C24-B04-320784	2
Fagron	Testosterone propionate	15I01-B01-318371	1
Fagron	Testosterone propionate	16E24-B01-322593	7
Caelo	Testosterone propionate	15444707	4
Caelo	Testosterone propionate	15444711	1
Fagron	Testosterone propionate	16E24-B01	1
Fagron	Testosterone propionate	16H22-B05	2
Euro OTC	Testosterone propionate	1512023-01	2
Fagron	Testosterone propionate	16H22-B05-326483	3
Fagron	Testosterone propionate	16H22-B05-326482	3
Caelo	Testosterone propionate	15444706	3
Fagro/Noweda	Testosterone propionate	16H22-B05-326483	2
Gehe	Testosterone propionate	15444706	1
Caelo	Testosterone propionate	15444712	1
Fagron	Testosterone propionate	16E24-B01-325476	1
Caelo	Testosterone propionate	15444710	2
Fagron	Testosterone propionate	16H22B05326483	1
Noweda	Testosterone propionate	1511003	1
Caelo	Testosterone propionate	16H22-B05-326483	1
Caelo	Testosterone propionate	15444719	1
Gehe/Fragon	Testosterone propionate	17B09B03332376	1
Fargon/Kehr	Testosterone propionate	17B09-B04-335269	1
Caelo	Testosterone propionate	15444714	2
Caelo	Testosterone propionate	15444717	1
Caelo	Testosterone propionate	1710027-01	1
Phoenix/Cealo	Testosterone propionate	36814M1	1
Euro OTC	Testosterone propionate	15444718	1
Fagron	Testosterone propionate	17B09-B03-332376	1
Audor Pharma	Testosterone propionate	APZTSP1503-MTP	1
Fagron	Testosterone propionate	17J16-B03-343010	1
Fagron	Testosterone propionate	17H25-B02-341321	1
Caelo	Testosterone propionate	15444721	1
Fagron	Testosterone propionate	17J16-B04-346529	1
Caelo	Testosterone propionate	17325707	2
Caelo	Testosterone propionate	15444718	1
Caelo	Testosterone propionate	18B14-B02-353456	1
Fagron	Testosterone propionate	18B06-B04-348557	1
Euro OTC	Testosterone propionate	1710027-01	1
Caelo	Testosterone propionate	17325719	1

- 78 611 spectra from 565 *Apo-Ident* customers from a total of 26 006 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Testosterone propionate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Testosterone propionate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	248	0	74 248
Type B	0	344	0	126 548
Type C	0	313	5	78 611

The substance/substance group *Testosterone propionate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5806 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.2558 %)
Type C	100.0000 % (> 99.8817 %)	98.4277 % (> 97.4843 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
22230	22230	0.00	8.93
23170	23170	0.00	6.09
20880	20880	0.00	7.08
22288	22288	0.00	7.77
21644	21644	0.00	8.86

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tetracaine base**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20947-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tetracaine base; Tetracainum

Special notes

When selecting the *Tetracaine base* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tetracaine base*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tetracaine base	12L19-N10	20947	40	20130108
Euro OTC	Tetracaine base	1405025-01	21603	40	AR-14-FG-012475-01
Fagron	Tetracaine base	14A16-B04-292915	21650	40	20140205
Fagron	Tetracaine base	14A16-B04-292916	21659	40	20140205
Euro OTC	Tetracaine base	1512022	22299	30	20160128*

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 190 spectra of 5 reference samples from the substance/substance group *Tetracaine base*. These samples are listed above in the [calibration samples](#) section.
- 74 306 spectra from a total of 1618 batches from further 372 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 [†].

- 535 spectra of 14 reference samples from the substance/substance group *Tetracaine base*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tetracaine base	1405025-01	21603 [†]	20
Fagron	Tetracaine base	14A16-B04-292915	21650 [†]	80
Fagron	Tetracaine base	14A16-B04-292916	21659 [†]	20
Euro OTC	Tetracaine base	1512022	22299 [†]	15
Euro OTC	Tetracaine base	1606009	22717	40
Euro OTC	Tetracaine base	1609010	22858	40
Euro OTC	Tetracaine base	1701035	23149	40
Caelo	Tetracaine base	171117	23321	40
Euro OTC	Tetracaine base	1708024	23736	40
Euro OTC	Tetracaine base	1803002	24066	40
Euro OTC	Tetracaine base	1805019	24135	40
Caelo	Tetracaine base	181249	24255	40
Euro OTC	Tetracaine base	1811021	24427	40
Euro OTC	Tetracaine base	1903004	24451	40

- 126 357 spectra from a total of 2775 batches from further 781 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.

- 145 spectra from 65 *Apo-Ident* customers from 72 batches from the substance/substance group *Tetracaine base*.

Supplier	Substance	Batch	Spectra
Phönix	Tetracaine base	11g12-n13	1
Fagron	Tetracaine base	12F29-N05	7
Phönix	Tetracaine base	3465093	1
Fagron	Tetracaine base	11L09-N03	3
Fagron	Tetracaine base	5111202	1
Fagron	Tetracaine base	12f29-n05	1
Fagron	Tetracaine base	12H23-N07	1
Fagron	Tetracaine base	11G12-N13	3
Fagron	Tetracaine base	11D07-N20	1
Fagron	Tetracaine base	12L19-N10	5
Fagron	Tetracaine base	12F26-N05	1
Caelo	Tetracaine base	T-290413-1	1
Fagron	Tetracaine base	11101-N09	1
Phönix	Tetracaine base	1303018-01	1
Fagron	Tetracaine base	13D30-N11	2
Fagron	Tetracaine base	3465093	1
Euro OTC	Tetracaine base	1312034-01	7
Fagron	Tetracaine base	14A16-B04-290209	1
GEHE 02.05.2014	Tetracaine base	14A16-B04-290208	2
Fagron	Tetracaine base	2913Q-07165	1
Fagron	Tetracaine base	14A16-B04-290208	3
Caelo	Tetracaine base	14A16-B04-292916	1
Fagron	Tetracaine base	TC0090913	2
Fagron	Tetracaine base	14A16-B04-292916	1
Phoenix 07.10.14	Tetracaine base	14A16-B04-292916	1
Phönix	Tetracaine base	1312034-01	1
Caelo	Tetracaine base	14A16-B04	1
Fagron	Tetracaine base	14G30-B08-297306	2
Fagron	Tetracaine base	14A16-B04-2490207	1
Euro OTC	Tetracaine base	1405025-01	1
Fagron	Tetracaine base	14G30-B08-297307	1
Phoenix Goettin	Tetracaine base	14G30-B08-297306	1
GEHE 04.05	Tetracaine base	1405025-01	1
Fagron	Tetracaine base	14G30-B08	2
Fagron	Tetracaine base	14g30-b08-297306	1
Fagron	Tetracaine base	14A16-B04	1
Fagron	Tetracaine base	14G30-B08-297305	1
Euro OTC	Tetracaine base	12081501	1
Fagron	Tetracaine base	14K03-B02-303179	2
Faron	Tetracaine base	15D01-B03-306258	2
Fagron	Tetracaine base	14g30-b08-297305	1
Fagron	Tetracaine base	14K03-B02	1
Euro OTC	Tetracaine base	151022-01	1
Fagron	Tetracaine base	15D01-B03-306258	1
Caelo	Tetracaine base	14A16-B04-290207	1
Fagron	Tetracaine base		1
Euro OTC	Tetracaine base	1512022-01	2

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Supplier	Substance	Batch	Spectra
Fagron	Tetracaine base	14a16-b04-290208	1
Euro OTC	Tetracaine base	1606009-01	6
Fagron	Tetracaine base	15/16-B06-312783	2
Caelo	Tetracaine base	16A13-B07-318736	4
Euro OTC	Tetracaine base	160600-01	1
Fagron	Tetracaine base	1516-B06-316259	1
Fagron	Tetracaine base	1516-B06-316260	1
Caelo	Tetracaine base	1512022-01	1
Caelo	Tetracaine base	1516B06312783	1
Caelo	Tetracaine base	16a13-b07-318736	1
Fagron	Tetracaine base	16A13-B07-318736	4
Fagron	Tetracaine base	15G30-B04-312060	1
Caelo	Tetracaine base	1606009-01	1
Fagron	Tetracaine base	15/16-B06-316260	1
Euro OTC	Tetracaine base	1609010-01	12
Caelo	Tetracaine base	16E23-B04	1
Hepart	Tetracaine base	15G30-B04-310590	1
Fagron	Tetracaine base	16E23-B04-323269	1
Fagron	Tetracaine base	14K03B02303178	1
Fagron	Tetracaine base	16G29B02325570	2
Fagron	Tetracaine base	16J12-B06	1
Euro OTC	Tetracaine base	160901	1
Fagron	Tetracaine base	16J12-B06-327371	1
Fagron	Tetracaine base	16G29-B02-325570	1
Euro OTC	Tetracaine base	1701035-01	4
Fagron	Tetracaine base	16A13-B07-322947	1
Ebert-Jacobi	Tetracaine base	16J12-B06-327371	1
GEHE	Tetracaine base	16G29-B02-325569	1
Euro OTC	Tetracaine base	3081701	1
Euro OTC	Tetracaine base	TC0091115	1
Fagron	Tetracaine base	16J12-B06-329087	1
Caelo	Tetracaine base	1701035-01	1
Fagron	Tetracaine base	16G29-B02-325569	1
Noweda/Fargon	Tetracaine base	16/12-B06-329087	1
Fagron	Tetracaine base	17E18-B02-337217	1
Euro OTC	Tetracaine base	1708024-01	2
Fagron	Tetracaine base	17E18-B02-337216	1
Euro OTC	Tetracaine base	18041809	1
Fagron	Tetracaine base	17K13-B02-344448	1
Caelo	Tetracaine base	17111705	1

- 78 784 spectra from 565 *Apo-Ident* customers from a total of 26 065 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tetracaine base* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tetracaine base* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	190	0	74 306
Type B	0	492	43	126 357
Type C	0	142	3	78 784

The substance/substance group *Tetracaine base* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.8421 %)
Type B	100.0000 % (> 99.9901 %)	91.9626 % (> 91.4019 %)
Type C	100.0000 % (> 99.8817 %)	97.9310 % (> 95.8621 %)

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
20947	21603	2.51	53.30
21603	21603	0.00	53.07
21650	22299	2.57	51.91
21659	21603	4.04	53.93
22299	22299	0.00	45.25

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tetracaine hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20037-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tetracaine hydrochloride; Tetracaini hydrochloridum

Special notes

When selecting the *Tetracaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tetracaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tetracaine hydro...	12019822	20924	40	20120228
Euro OTC	Tetracaine hydro...	1506040	21845	40	20150713*
Euro OTC	Tetracaine hydro...	1512019	22285	30	20151228*
Euro OTC	Tetracaine hydro...	1612005	22912	40	20170112*
Fagron	Tetracaine hydro...	15K04-B03-322151	23162	40	20160112
Caelo	Tetracaine hydro...	15437108	23163	40	20160211
Euro OTC	Tetracaine hydro...	1807017	24141	40	20180730*

Validation samples

A total of 280317 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 *Tetracaine hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74226 spectra from a total of 1616 batches from further 372 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 [†].

- 355 spectra of 10 reference samples from the substance/substance group *Tetracaine hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tetracaine hydrochloride	1506040	21845 [†]	20
Euro OTC	Tetracaine hydrochloride	1512019	22285 [†]	15
Euro OTC	Tetracaine hydrochloride	1607031	22708	40
Fagron	Tetracaine hydrochloride	16G28-B03-327368	23500	40
Euro OTC	Tetracaine hydrochloride	1706018	23558	40
Euro OTC	Tetracaine hydrochloride	1712012	23886	40
Euro OTC	Tetracaine hydrochloride	1310006	23910	40
Euro OTC	Tetracaine hydrochloride	1803001	24079	40
Euro OTC	Tetracaine hydrochloride	1812006	24448	40
Euro OTC	Tetracaine hydrochloride	1902015	24452	40

- 126537 spectra from a total of 2779 batches from further 781 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.

- 697 spectra from 253 *Apo-Ident* customers from 179 batches from the substance/substance group *Tetracaine hydrochloride*.

Supplier	Substance	Batch	Spectra
EuRho	Tetracaine hydrochloride	1110010-01	2
Caelo	Tetracaine hydrochloride	10118225	4
Caelo	Tetracaine hydrochloride	12019802	4
Euro OTC	Tetracaine hydrochloride	1110010-01	5
Caelo	Tetracaine hydrochloride	9070003	2
Finze	Tetracaine hydrochloride	2906009-02	1
Euro OTC	Tetracaine hydrochloride	1110010-02	6
Fagron	Tetracaine hydrochloride	12C22-N04	5
Caelo	Tetracaine hydrochloride	10118211	1
Noweda	Tetracaine hydrochloride	1106035-01	2
Caelo	Tetracaine hydrochloride	1110010-02	2
Fagron	Tetracaine hydrochloride	11A31-N15	1
Fagron	Tetracaine hydrochloride	11C22-N04	1
Caelo	Tetracaine hydrochloride	10118210	2
Euro OTC	Tetracaine hydrochloride	20160812-2	1
EuRho	Tetracaine hydrochloride	2906009V-04	1
Fagron	Tetracaine hydrochloride	12H24-N05	11
Caelo	Tetracaine hydrochloride	12019812	3
Euro OTC	Tetracaine hydrochloride	11110010-02	1
Euro OTC	Tetracaine hydrochloride	1207001-01	8
Caelo	Tetracaine hydrochloride	1110010-01	1
EuRho	Tetracaine hydrochloride	1106035-01	2
Caelo	Tetracaine hydrochloride	1207001-01	1
Fagron	Tetracaine hydrochloride	12H-N05	1
Caelo	Tetracaine hydrochloride	12019810	5
Fagron	Tetracaine hydrochloride	10A29-N12	2
Caelo	Tetracaine hydrochloride	12019816	11
Noweda	Tetracaine hydrochloride	120700-02	1
Fagron	Tetracaine hydrochloride	12K01-N04	7
Noweda/ BASF Pharma (Ev...	Tetracaine hydrochloride	12H24-N05	1
Euro OTC	Tetracaine hydrochloride	2906009V-03	1
Fagron	Tetracaine hydrochloride	13D11-N07	11
Euro OTC	Tetracaine hydrochloride	1207001-02	8
Caelo	Tetracaine hydrochloride	12019815	1
Jenne	Tetracaine hydrochloride	13D11-No7	1
Alliance Healthcare	Tetracaine hydrochloride	12H24-N05	1
EuRho Anzag	Tetracaine hydrochloride	1207001-01	1
Fagron	Tetracaine hydrochloride	3413U02039	1
Euro OTC	Tetracaine hydrochloride	1303012-01	21
Sino Phyto	Tetracaine hydrochloride	12019816	1
Fagron	Tetracaine hydrochloride	3913I-02039	1
Fagron	Tetracaine hydrochloride	1303012-01	1
Fagron	Tetracaine hydrochloride	4313E-02039	1
Fagron	Tetracaine hydrochloride	12H24-N050696/1050	1
Fagron	Tetracaine hydrochloride	11/15-N12	1
Caelo	Tetracaine hydrochloride	12019822	6
Orgamol Pharma	Tetracaine hydrochloride	6093547	1
Euro OTC	Tetracaine hydrochloride	130301201	1
Noveda	Tetracaine hydrochloride	12H24-N05	1
Phönix	Tetracaine hydrochloride	130301201	1
Caelo	Tetracaine hydrochloride	12019820	1
Fagron	Tetracaine hydrochloride	13D11-N01	1

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Supplier	Substance	Batch	Spectra
Euro CT Phönix	Tetracaine hydrochloride	1207001-02	1
Caelo	Tetracaine hydrochloride	27111305	1
Fagron	Tetracaine hydrochloride	212131/221630-0002	1
Euro OTC	Tetracaine hydrochloride	6093547	1
Fagron	Tetracaine hydrochloride	13G02-N01	1
Euro OTC	Tetracaine hydrochloride	1310006-01	18
Caelo	Tetracaine hydrochloride	1313012-01	1
Caelo	Tetracaine hydrochloride	12H24-N05	1
Sanacorp	Tetracaine hydrochloride	1207001-02	1
Sanacorp	Tetracaine hydrochloride	1303012-01	1
Gehe	Tetracaine hydrochloride	1310006-01	1
BASF Pharma S.A.	Tetracaine hydrochloride	1310006-01	1
Caelo	Tetracaine hydrochloride	13155706	10
Euro OTC	Tetracaine hydrochloride	13155710	4
Gutenberg-Apotheke	Tetracaine hydrochloride	13D11-N07	1
Phoenix am 30.04.2014	Tetracaine hydrochloride	1310006-01	1
Alliance Health 30.04.2...	Tetracaine hydrochloride	1303012-01	2
Alliance Health 05.05.2...	Tetracaine hydrochloride	13H21-B02-286559	1
Fagron	Tetracaine hydrochloride	6093547	2
Fagron	Tetracaine hydrochloride	13H21-B02-286558	3
EuroTOC / Noweda	Tetracaine hydrochloride	131000601	2
Fagron	Tetracaine hydrochloride	13H21-B02	2
Euro OTC	Tetracaine hydrochloride		1
Caelo	Tetracaine hydrochloride	13155705	3
Fagron	Tetracaine hydrochloride	13K25-B04-290276	2
Sanacorp	Tetracaine hydrochloride	15/AKD1	1
Fagron	Tetracaine hydrochloride		1
Caelo	Tetracaine hydrochloride	1310006-01	1
Caelo	Tetracaine hydrochloride	13155711	7
Noweda	Tetracaine hydrochloride	1310006-01	1
Caelo	Tetracaine hydrochloride	6093549	1
Euro OTC	Tetracaine hydrochloride	1405026-01	16
euroct/gehe	Tetracaine hydrochloride	1405026-01	1
Fagron	Tetracaine hydrochloride	13K25-B04290276	1
Gehe 07.07.2014	Tetracaine hydrochloride	13155706	1
Fagron	Tetracaine hydrochloride	13H21-B02-286559	1
Caelo	Tetracaine hydrochloride	1405026-01	1
Gatt-Koller / Phoenix	Tetracaine hydrochloride	80/02140614	2
Alliance Health 22.08.2...	Tetracaine hydrochloride	6093549	1
Caelo	Tetracaine hydrochloride	13K25-B04-290276	1
Bombastus	Tetracaine hydrochloride	13H21-B02-286558	1
Euro OTC	Tetracaine hydrochloride	140502601	1
Euro OTC	Tetracaine hydrochloride	24102014A	1
Fagron	Tetracaine hydrochloride	14C18-B03-293966	7
VDI 26.09.14 12,00 euro	Tetracaine hydrochloride	1405026-01	1
Euro OTC	Tetracaine hydrochloride	1409026-01	11
Fagron	Tetracaine hydrochloride	10990834	3
Fagron	Tetracaine hydrochloride	13155711	1
Synopharm/Anzag	Tetracaine hydrochloride	2712Q-02039	1
Caelo	Tetracaine hydrochloride	14c18-b03-293966	1
Fagron	Tetracaine hydrochloride	13K25-B04	1
Euro OTC	Tetracaine hydrochloride	1411019-01	21
Euro OTC	Tetracaine hydrochloride	14090-26	1
Gehe	Tetracaine hydrochloride	13155711	2
Euro OTC	Tetracaine hydrochloride	1409026	1
Caelo	Tetracaine hydrochloride	13155720	2
Euro OTC	Tetracaine hydrochloride	1106035-01	1
Sanacorp	Tetracaine hydrochloride	1409026-01	1
Fagron	Tetracaine hydrochloride	6093549	1
Euro OTC	Tetracaine hydrochloride	14G14-B08-300202	1

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Supplier	Substance	Batch	Spectra
Alliance Health	Tetracaine hydrochloride	14C18-B03-293967	1
Caelo	Tetracaine hydrochloride	13155716	2
Phoenix Goettin	Tetracaine hydrochloride	1409026-01	1
Euro OTG	Tetracaine hydrochloride	1207001-01	1
Fagron	Tetracaine hydrochloride	14c18d03300199	1
Caelo	Tetracaine hydrochloride	1411019-01	4
Fagron	Tetracaine hydrochloride	13K25-B04-290278	1
Fagron	Tetracaine hydrochloride	13k25-b04-290276	1
Fagron	Tetracaine hydrochloride	14C18-B03-300199	4
Caelo	Tetracaine hydrochloride	15079501	2
Euro OTC	Tetracaine hydrochloride	1411019	1
Caelo	Tetracaine hydrochloride	13155724	4
Euro OTC	Tetracaine hydrochloride	140902601	1
Caelo	Tetracaine hydrochloride	13155714	2
Fagron	Tetracaine hydrochloride	1418-03-300199	1
Fagron	Tetracaine hydrochloride	14G14-B08-300198	5
Euro OTC	Tetracaine hydrochloride	141101901	1
Caelo	Tetracaine hydrochloride	13155727	5
Caelo	Tetracaine hydrochloride	13155703	1
Fagron	Tetracaine hydrochloride	10990837	3
Caelo	Tetracaine hydrochloride	14C18-B03-300200	1
Fagron	Tetracaine hydrochloride	14C18-B03-293967	1
Fagron	Tetracaine hydrochloride	10330837	1
Euro OTC	Tetracaine hydrochloride	17081503	1
Calo/AHD	Tetracaine hydrochloride	13155727	1
Fagron	Tetracaine hydrochloride	14C18-B03-300200	4
BASF Pharma	Tetracaine hydrochloride	1411019-01	1
Fagron	Tetracaine hydrochloride	1411019-01	1
Euro OTC	Tetracaine hydrochloride	1409026-02	9
Caelo	Tetracaine hydrochloride	1409026-02	3
Fagron	Tetracaine hydrochloride	13K25-Bo4-290276	1
Fagron	Tetracaine hydrochloride	15A12-B03-308857	6
BASF Fine Chemicals Swi...	Tetracaine hydrochloride	13155714	1
Caelo	Tetracaine hydrochloride	14C18-B03-300199	1
Fagron	Tetracaine hydrochloride	14C18-Bo3-300200	1
BASF Pharma S.A.	Tetracaine hydrochloride	1409026-02	1
Caelo	Tetracaine hydrochloride	14G14-B08-300198	1
Euro OTC	Tetracaine hydrochloride	1506040-01	24
Euro/Phönix	Tetracaine hydrochloride	1506040-01	1
Euro OTG Pharma	Tetracaine hydrochloride	1409026-02	1
Caelo	Tetracaine hydrochloride	15196102	4
Fagron	Tetracaine hydrochloride	10990841	1
Euro OTC	Tetracaine hydrochloride	150604001	1
Anzag	Tetracaine hydrochloride	1411019-01	1
Euro	Tetracaine hydrochloride	1506040-01	1
Euro OTC	Tetracaine hydrochloride	3113M-02039	1
Caelo	Tetracaine hydrochloride	15196103	5
Caelo	Tetracaine hydrochloride	14G14-B08	1
Caelo	Tetracaine hydrochloride	15H24-B03-311450	1
AHD	Tetracaine hydrochloride	15A12-B03-308857	1
Fagron	Tetracaine hydrochloride	15H24-B03-311450	6
Caelo	Tetracaine hydrochloride	150604001	1
Caelo	Tetracaine hydrochloride	15079507	1
Euro OTC	Tetracaine hydrochloride	4811A-02039	1
Caelo	Tetracaine hydrochloride	15196104	2
Euro OTC	Tetracaine hydrochloride	1512019-01	26
Fagron	Tetracaine hydrochloride	14C18-B03	1
Phoenix	Tetracaine hydrochloride	15437104	2
EuRho	Tetracaine hydrochloride	1615I-02039	1
Caelo	Tetracaine hydrochloride	15356902	2

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Supplier	Substance	Batch	Spectra
Fagron	Tetracaine hydrochloride	15H24-B03	3
Fagron	Tetracaine hydrochloride	15H24-B03-313594	5
Caelo	Tetracaine hydrochloride	15437104	13
Fagron	Tetracaine hydrochloride	15h24-b03-313594	1
Caelo	Tetracaine hydrochloride	15437102	1
Caelo	Tetracaine hydrochloride	15437106	2
Euro OTC	Tetracaine hydrochloride	1506040-02	7
Euro OTC	Tetracaine hydrochloride	15120019-01	1
Euro OTC	Tetracaine hydrochloride	10416THCL	1
Fagron	Tetracaine hydrochloride	15K04B03318369	1
Fagron	Tetracaine hydrochloride	15K04-B03-318368	3
Caelo	Tetracaine hydrochloride	15K04-B03-318368	2
Fargon Services NL	Tetracaine hydrochloride	15K04-B03-322151	5
Phönix	Tetracaine hydrochloride	2015E-02039	1
Euro OTC	Tetracaine hydrochloride	13509155	1
Caelo	Tetracaine hydrochloride	15437109	9
Euro OTC	Tetracaine hydrochloride	1607031-01	26
Euro OTC	Tetracaine hydrochloride	151-2019-01	1
Euro OTC	Tetracaine hydrochloride	1512019-02	1
Phoenix 04.11.16 Phoeni...	Tetracaine hydrochloride	1607031-01	1
Caelo	Tetracaine hydrochloride	15437108	1
Caelo	Tetracaine hydrochloride	1512019-02	1
Fagron	Tetracaine hydrochloride	15K04-B03-322151	6
Caelo	Tetracaine hydrochloride	15K04-B03-318369	1
Fagron	Tetracaine hydrochloride	15K04-bo3-312151	1
Euro OTC	Tetracaine hydrochloride	1405026-02	1
Phönix	Tetracaine hydrochloride	1405026-01	1
Sanacorp, 21.02.17, 13,...	Tetracaine hydrochloride	1607031-01	1
Fagron	Tetracaine hydrochloride	16G28-B03-327369	2
Fagron	Tetracaine hydrochloride	16G28-B03-327368	7
Gehe	Tetracaine hydrochloride	15K04-B03-322151	1
Caelo	Tetracaine hydrochloride	1607031-01	5
Caelo	Tetracaine hydrochloride	1110010-07	1
Fagron	Tetracaine hydrochloride	1607031-01	1
Euro OTC	Tetracaine hydrochloride	1612005-01	14
Euro OTC	Tetracaine hydrochloride	1405026-04	1
Noweda	Tetracaine hydrochloride	14G14-B08	1
Fagron	Tetracaine hydrochloride	15K04-B03322151	1
Euro OTC	Tetracaine hydrochloride	1607031	1
Euro OTC	Tetracaine hydrochloride	1607032-01	1
Ebert-Jacobi	Tetracaine hydrochloride	1612005-01	1
Ebert-Jacobi	Tetracaine hydrochloride	15K04-B03-328163	1
Euro OTC	Tetracaine hydrochloride	3071716	1
Caelo	Tetracaine hydrochloride	15437114	5
Fagron	Tetracaine hydrochloride	16G28-B03-330363	1
Fagro/Gehe	Tetracaine hydrochloride	16G28-B03-327368	2
Anzag	Tetracaine hydrochloride	14710369	1
Caelo	Tetracaine hydrochloride	15437119	6
GEHE	Tetracaine hydrochloride	1612005-01	1
Euro OTG/ AHD	Tetracaine hydrochloride	1706018-01	2
Caelo	Tetracaine hydrochloride	16G25-B03-332099	1
Caelo	Tetracaine hydrochloride	1508040-01	1
Fagron	Tetracaine hydrochloride	16G28-B03-334124	2
Caelo	Tetracaine hydrochloride	1260917/15437119	1
Caelo	Tetracaine hydrochloride	15437122	1
Caelo	Tetracaine hydrochloride	15437121	3
Caelo	Tetracaine hydrochloride	1612005-01	1
GEHE	Tetracaine hydrochloride	1706018-01	1
Bomastus / Alliance Hea...	Tetracaine hydrochloride	16G28-B03-327368	2
Euro OTC	Tetracaine hydrochloride	1612005-015445	1

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Supplier	Substance	Batch	Spectra
Caelo	Tetracaine hydrochloride	16G28-B03-332099	1
Euro OT/Phönix	Tetracaine hydrochloride	TH0030315	1
Fagron	Tetracaine hydrochloride	17G03-B07-338538	4
Fagron	Tetracaine hydrochloride	218I-02039	1
Phönix	Tetracaine hydrochloride	1612005-01	1
Fagron	Tetracaine hydrochloride	17G03-B07	2
Euro OTC	Tetracaine hydrochloride	TH0030315	1
Euro OTC	Tetracaine hydrochloride	1712012-01	5
AHD	Tetracaine hydrochloride	15437121	1
Bombastus	Tetracaine hydrochloride	1712012-01	2
Fagron	Tetracaine hydrochloride	17G03-B07-338539	2
Anzag	Tetracaine hydrochloride	17256705	1
Euro OTC	Tetracaine hydrochloride	1310006-02	1
Euro OTC	Tetracaine hydrochloride	1706018-01	2
Fagron	Tetracaine hydrochloride	17G03-B07-338540	1
Fagron	Tetracaine hydrochloride	17G03-B07-341319	1
Euro OTC	Tetracaine hydrochloride	21071807	1
Caelo	Tetracaine hydrochloride	18060602	2
Caelo	Tetracaine hydrochloride	17256705	1
Fagron	Tetracaine hydrochloride	17G03-B07-341853	1
Sanacorp	Tetracaine hydrochloride	17G03-B07-341853	1
Euro OTC	Tetracaine hydrochloride	1807017-01	1
Caelo	Tetracaine hydrochloride	17G03-B07-345008	1
Euro OTC	Tetracaine hydrochloride	18701701	1
Fagron	Tetracaine hydrochloride	17G03-B07-349368	1
Euro OTC	Tetracaine hydrochloride	1803001-01	5
Euro OTC	Tetracaine hydrochloride	180300101	1
Caesar & Loretz	Tetracaine hydrochloride	1803001-01	1
Euro OTC	Tetracaine hydrochloride	1812006-01	2

- 78 232 spectra from 565 *Apo-Ident* customers from a total of 25 960 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tetracaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tetracaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 226
Type B	0	355	0	126 537
Type C	0	692	5	78 232

The substance/substance group *Tetracaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.3099 %)
Type C	100.0000 % (> 99.8817 %)	99.2826 % (> 98.8522 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22912	22912	0.00	66.01
23162	22912	3.92	65.94
20924	22912	3.23	66.01
21845	21845	0.00	64.06
22285	22285	0.00	63.83
23163	21845	5.51	65.36
24141	24141	0.00	61.09

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tetracycline hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20044-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tetracycline hydrochloride; Tetracyclini hydrochloridum

Special notes

When selecting the *Tetracycline hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tetracycline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tetracycline hyd...	1302012-01	21079	40	1411585
Caelo	Tetracycline hyd...	13201303	21427	40	20130807
Caelo	Tetracycline hyd...	13201303	21428	40	20130807
Euro OTC	Tetracycline hyd...	1506012	21835	40	20150707*
Caelo	Tetracycline hyd...	161167	22468	40	20160504*
Caelo	Tetracycline hyd...	15230712	22833	40	20150819

Validation samples

A total of 280317 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 *Tetracycline hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74256 spectra from a total of 1618 batches from further 372 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 [†].

- 310 spectra of 10 reference samples from the substance/substance group *Tetracycline hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tetracycline hydrochloride	13201303	21427 [†]	20
Caelo	Tetracycline hydrochloride	13201303	21428 [†]	20
Euro OTC	Tetracycline hydrochloride	1506012	21835 [†]	20
Caelo	Tetracycline hydrochloride	161167	22468 [†]	20
Euro OTC	Tetracycline hydrochloride	1603026	22545	40
Euro OTC	Tetracycline hydrochloride	1706020	23691	30
Caelo	Tetracycline hydrochloride	172858	23847	40
Caelo	Tetracycline hydrochloride	181986	24256	40
Caelo	Tetracycline hydrochloride	183083	24394	40
Euro OTC	Tetracycline hydrochloride	1811031	24450	40

- 126582 spectra from a total of 2780 batches from further 781 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.

- 305 spectra from 156 *Apo-Ident* customers from 102 batches from the substance/substance group *Tetracycline hydrochloride*.

Supplier	Substance	Batch	Spectra
Caelo	Tetracycline hydrochloride	5091202	1
Euro OTC	Tetracycline hydrochloride	1103003-01	1
Gehe	Tetracycline hydrochloride	1110029-01	1
Euro OTC	Tetracycline hydrochloride	1110029-01	2
Caelo	Tetracycline hydrochloride	9248704	1
Caelo	Tetracycline hydrochloride	111002901	1
Caelo	Tetracycline hydrochloride	1204039	2
Fagron	Tetracycline hydrochloride	12E10-N05	1
Euro OTC	Tetracycline hydrochloride	1204039-01	5
Caelo	Tetracycline hydrochloride	12138106	2
Euro OTC	Tetracycline hydrochloride	100518-62	1
Euro OTC	Tetracycline hydrochloride	28021315	1
Caelo	Tetracycline hydrochloride	12353602	1
Euro OTC	Tetracycline hydrochloride	12040390	1
Europharm/Otto	Tetracycline hydrochloride	1204039-01	1
Fagron	Tetracycline hydrochloride	12J15-N05	1
Caelo	Tetracycline hydrochloride	12353603	6
Europharm/Otto	Tetracycline hydrochloride	1204039-02	3
Euro OTC	Tetracycline hydrochloride	1204039-02	11
Eurho/Phoenix	Tetracycline hydrochloride	1204039-02	1
Caelo	Tetracycline hydrochloride	12138104	1
Caelo	Tetracycline hydrochloride	12353609	1
Sanacorp	Tetracycline hydrochloride	100403401	1
Euro OTC	Tetracycline hydrochloride	120403902	1
Euro OTC	Tetracycline hydrochloride	1302012-01	7
Fagron	Tetracycline hydrochloride	13F17-N03	4
Caelo	Tetracycline hydrochloride	1302012-01	1
Phönix Gotha	Tetracycline hydrochloride	1302012-01	1
Euro OTC	Tetracycline hydrochloride	1302012-02	15
Caelo	Tetracycline hydrochloride	12353612	1
EUro/AHD	Tetracycline hydrochloride	1302012-01	1
Aliance am 10.03.2014	Tetracycline hydrochloride	1302012-02	1
Caelo	Tetracycline hydrochloride	13F17-N03	1
Caelo	Tetracycline hydrochloride	13201301	3
Caelo	Tetracycline hydrochloride	103201301	1
Fagron	Tetracycline hydrochloride	13J22-N04	1
Fagron	Tetracycline hydrochloride	13201301	1
Caelo	Tetracycline hydrochloride	4012Q-02378	1
Caelo	Tetracycline hydrochloride	13201302	1
Caelo	Tetracycline hydrochloride	1402030-01	1
Caelo	Tetracycline hydrochloride	12353613	1
Euro OTC	Tetracycline hydrochloride	1402030-01	8
Fagron	Tetracycline hydrochloride	13L10-B02-294455	2
EuRho	Tetracycline hydrochloride	1302012-02	1
Alliance Health 22.08.2...	Tetracycline hydrochloride	13201307	1
EuRho	Tetracycline hydrochloride	1402030-02	1
Euro OTC	Tetracycline hydrochloride	140203001	1
Euro OTC	Tetracycline hydrochloride	1402030-02	7
Fagron	Tetracycline hydrochloride	1402030-02	2
Celo/Kehr	Tetracycline hydrochloride	13201307	1
Euro OTC	Tetracycline hydrochloride	21111404	1
Caelo	Tetracycline hydrochloride	13L10B02296956	1

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Supplier	Substance	Batch	Spectra
Caelo	Tetracycline hydrochloride	13201307	1
Fagron	Tetracycline hydrochloride	13L10-B02-294454	1
Sanacorp	Tetracycline hydrochloride	1402030-01	1
Caelo	Tetracycline hydrochloride	13201309	1
Caelo	Tetracycline hydrochloride	14080605	2
Euro OTC	Tetracycline hydrochloride	1412007-01	9
Euro OTC	Tetracycline hydrochloride	13042015C	1
Fagron	Tetracycline hydrochloride	14H06-B05-299498	1
Euro OTC	Tetracycline hydrochloride	140410-62	1
Fagron	Tetracycline hydrochloride	14H06-B05-303911	1
Caelo	Tetracycline hydrochloride	1412007-01	2
Caelo	Tetracycline hydrochloride	14080606	3
Fagron	Tetracycline hydrochloride	14H06-B05-303912	6
Caelo	Tetracycline hydrochloride	14364604	3
Euro OTC	Tetracycline hydrochloride	141200701	1
Noweda	Tetracycline hydrochloride	13201307	1
Anzag/euRho	Tetracycline hydrochloride		1
Euro OTC	Tetracycline hydrochloride	1506012-01	22
EuRho/AHD	Tetracycline hydrochloride		1
Hoff/ Noweda	Tetracycline hydrochloride	14364604	1
Euro OTC	Tetracycline hydrochloride	14120007-01	1
Caelo	Tetracycline hydrochloride	2714U-02378	1
Fagron	Tetracycline hydrochloride	14H06-Bo5-303912	1
ningxia	Tetracycline hydrochloride	1412007-01	1
Caelo	Tetracycline hydrochloride	14364612	2
Caelo	Tetracycline hydrochloride	14364614	1
Fagron	Tetracycline hydrochloride	14H06-B05	1
Caelo	Tetracycline hydrochloride	14364616	2
Caelo	Tetracycline hydrochloride	14H06-B05-313591	1
Fagron	Tetracycline hydrochloride	1506012-01	1
Fagron	Tetracycline hydrochloride	14H06-B05-311707	1
Gehe	Tetracycline hydrochloride	15230703	1
Fagron	Tetracycline hydrochloride	14H06-B05-314870	1
Caelo	Tetracycline hydrochloride	15230703	3
Euro OTC	Tetracycline hydrochloride	150601201	2
Caelo	Tetracycline hydrochloride	1506012-01	1
Bombastus	Tetracycline hydrochloride	1204039-02	1
Caelo	Tetracycline hydrochloride	15230707	2
Euro OTC	Tetracycline hydrochloride	1603026-01	26
Caelo	Tetracycline hydrochloride	1603026-01	3
Euro OTC	Tetracycline hydrochloride	160621TCH	1
Caelo	Tetracycline hydrochloride	15230717	2
Bombastus	Tetracycline hydrochloride	1603026-01	2
Caelo	Tetracycline hydrochloride	4315I-02378	1
Ningxia	Tetracycline hydrochloride	1603026-01	3
Caelo	Tetracycline hydrochloride	15230720	2
Euro OTC	Tetracycline hydrochloride	160302601	2
Euro OTC	Tetracycline hydrochloride	1603026	1
Caelo	Tetracycline hydrochloride	15230715	2
Caelo	Tetracycline hydrochloride	16116701	3
Ichthyl/Phönix	Tetracycline hydrochloride	1603026-01	1
Caelo	Tetracycline hydrochloride	1160117	1
Caelo	Tetracycline hydrochloride	15230711	1
Ichthyl-Gesellschaft	Tetracycline hydrochloride	1603026-01	1
Caelo	Tetracycline hydrochloride	16116706	3
Euro OTC	Tetracycline hydrochloride	21031702	1
Gehe	Tetracycline hydrochloride	16116706	1
Caelo	Tetracycline hydrochloride	1017A-02378	1
Caelo	Tetracycline hydrochloride	16116704	1
Caelo	Tetracycline hydrochloride	16116709	2

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Supplier	Substance	Batch	Spectra
Euro OTC	Tetracycline hydrochloride	1412007-03	4
Euro OTC	Tetracycline hydrochloride	1506012-02	2
Euro OTC	Tetracycline hydrochloride	27101708	1
Caelo	Tetracycline hydrochloride	166116709	1
Jenne	Tetracycline hydrochloride	1506012-02	1
Euro OTC	Tetracycline hydrochloride	1506012-02Eur	1
Caelo	Tetracycline hydrochloride	16116714	1
Euro OTC	Tetracycline hydrochloride	160302	1
Euro OTC	Tetracycline hydrochloride	411682	1
Caelo	Tetracycline hydrochloride	16116720	1
s. Protokoll	Tetracycline hydrochloride		1
Caelo	Tetracycline hydrochloride	16116715	2
Euro OTC	Tetracycline hydrochloride	180306T/1412007-03	1
Noweda	Tetracycline hydrochloride	1412007-03	1
Caelo	Tetracycline hydrochloride	16116721	1
Caelo	Tetracycline hydrochloride	17285801	2
Euro OTC	Tetracycline hydrochloride	1706020-01	11
Euro OTC	Tetracycline hydrochloride	17060201-01	1
Euro OTG/ AHD	Tetracycline hydrochloride	1706020-01	1
Caelo	Tetracycline hydrochloride	17285803	3
Caelo	Tetracycline hydrochloride	172855809	1
Caelo	Tetracycline hydrochloride	17285809	3
Caelo	Tetracycline hydrochloride	18198602	1
Jenne	Tetracycline hydrochloride	18198602	1

- 78 624 spectra from 565 *Apo-Ident* customers from a total of 26 036 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tetracycline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tetracycline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	310	0	126 582
Type C	0	297	8	78 624

The substance/substance group *Tetracycline hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.0645 %)
Type C	100.0000 % (> 99.9817 %)	97.3770 % (> 96.3934 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21079	21079	0.00	25.03
21427	21079	7.32	27.69
22833	21079	6.97	26.62
21428	21835	2.81	28.19
21835	21835	0.00	27.16
22468	22468	0.00	25.72

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Thalidomide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21552-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Thalidomide; Thalidomidum

Special notes

When selecting the *Thalidomide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Thalidomide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Thalidomide	14E27B04295348	21552	40	1503608
Caelo	Thalidomide	15276711	22880	40	1704508
Fagron	Thalidomide	15A13-B01-312230	22882	40	1704509
Caelo	Thalidomide	182496	24399	40	20181022*

Validation samples

A total of 280 317 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 *Thalidomide*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Thalidomide*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Thalidomide	14E27B04295348	21552 [†]	20
Caelo	Thalidomide	13395704	21739	60
Caelo	Thalidomide	162703	22774	40
Caelo	Thalidomide	172100	23684	40

- 126 732 spectra from a total of 2785 batches from further 781 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*.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Thalidomide*.

Supplier	Substance	Batch	Spectra
Fagron	Thalidomide	14E27-B04-299297	1
Fagron	Thalidomide	13K20-N01	1

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Thalidomide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Thalidomide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	60	100	126 732
Type C	0	0	2	78 927

The substance/substance group *Thalidomide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	37.5000 % (> 35.6250 %)
Type C	100.0000 % (> 99.8823 %)	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
21552	21552	0.00	50.11
22880	22880	0.00	52.86
24399	24399	0.00	59.13
22882	22882	0.00	69.39

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Theophylline**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20723-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Theophylline; Theophyllinum

Special notes

When selecting the *Theophylline* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Theophylline*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Theophylline	12166316	20723	40	1402055
Caelo	Theophylline	12341101	21740	40	20121115

Validation samples

A total of 280 317 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 *Theophylline*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Theophylline*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Theophylline	12341101	21740 [†]	20
Caelo	Theophylline	15203018	23253	40
Caelo	Theophylline	171962	23854	40

- 126 792 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 13 spectra from 12 *Apo-Ident* customers from 9 batches from the substance/substance group *Theophylline*.

Supplier	Substance	Batch	Spectra
Noweda	Theophylline	12166305	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	Theophylline	12166312	1
Caelo	Theophylline	12166305	2
Caesar&lorenz,Phoenix	Theophylline	12166315	1
Caelo	Theophylline	12166315	1
Caelo	Theophylline	12166311	1
Caelo	Theophylline	12166306	1
Caelo	Theophylline	12341101	2
Caelo	Theophylline	12341104	1
Caelo	Theophylline	17196203	1
Caelo	Theophylline	15203010	1

- 78 916 spectra from 565 *Apo-Ident* customers from a total of 26 128 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Theophylline* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Theophylline* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	100	0	126 792
Type C	0	11	2	78 916

The substance/substance group *Theophylline* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8818 %)	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
20723	20723	0.00	52.77
21740	20723	9.79	56.47

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Theophylline-ethylenediamine hydrate
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20831-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Theophylline-ethylenediamine hydrate; Theophyllinum et ethylenediaminum hydricum

Special notes

When selecting the *Theophylline-ethylenediamine hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Theophylline-ethylenediamine hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Theophylline-eth...	12145301	20831	40	20120628
Caelo	Theophylline-eth...	12363708	20992	40	20130116
Caelo	Theophylline-eth...	13268609	21549	40	1412133

Validation samples

A total of 280 317 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 *Theophylline-ethylenediamine hydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 4 reference samples from the substance/substance group *Theophylline-ethylenediamine hydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Theophylline-ethylenediamine...	15380302	22589	40
Caelo	Theophylline-ethylenediamine...	17073707	23564	30
Caelo	Theophylline-ethylenediamine...	172999	23823	40
Caelo	Theophylline-ethylenediamine...	182738	24383	40

- 126 742 spectra from a total of 2785 batches from further 781 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 *Theophylline-ethylenediamine hydrate*.

Supplier	Substance	Batch	Spectra
ACM / Phoenix	Theophylline-ethylenediamine...	KNC0896J14	1
Caelo	Theophylline-ethylenediamine...	15380302	1

- 78 927 spectra from 565 *Apo-Ident* customers from a total of 26 135 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Theophylline-ethylenediamine hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Theophylline-ethylenediamine hydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	150	0	126 742
Type C	0	2	0	78 927

The substance/substance group *Theophylline-ethylenediamine hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.8823 %)	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
20831	21549	4.66	61.45
20992	21549	1.76	62.93
21549	21549	0.00	63.34

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Thiamine chloride hydrochloride
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20566-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Thiamine chloride hydrochloride; Aneurinum hydrochloricum

Special notes

When selecting the *Thiamine chloride hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Thiamine chloride hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Thiamine chlorid. ...	14069502	21511	40	8986
Euro OTC	Thiamine chlorid. ...	1211008-02	21647	40	20121122
Caelo	Thiamine chlorid. ...	160156	22477	40	20160316*
Euro OTC	Thiamine chlorid. ...	1612004	22919	40	20170117*

Validation samples

A total of 280 317 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 *Thiamine chloride hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 [†].

- 280 spectra of 8 reference samples from the substance/substance group *Thiamine chloride hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Thiamine chloride hydrochlor...	14069502	21478	60
Caelo	Thiamine chloride hydrochlor...	14069502	21511 [†]	20
Euro OTC	Thiamine chloride hydrochlor...	1211008-02	21647 [†]	20
Caelo	Thiamine chloride hydrochlor...	160156	22477 [†]	20
Caelo	Thiamine chloride hydrochlor...	170976	23368	40
Euro OTC	Thiamine chloride hydrochlor...	1705034	23439	40
Euro OTC	Thiamine chloride hydrochlor...	1712013	23911	40
Euro OTC	Thiamine chloride hydrochlor...	1807001	24146	40

- 126 612 spectra from a total of 2782 batches from further 781 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.

- 33 spectra from 14 *Apo-Ident* customers from 24 batches from the substance/substance group *Thiamine chloride hydrochloride*.

Supplier	Substance	Batch	Spectra
Finze	Thiamine chloride hydrochlor...	9216114	1
Caelo	Thiamine chloride hydrochlor...	11371309	2
Euro OTC	Thiamine chloride hydrochlor...	1211008-01	1
Caelo	Thiamine chloride hydrochlor...	11371319	3
Caelo	Thiamine chloride hydrochlor...	11371313	1
Caelo	Thiamine chloride hydrochlor...		1
Caelo	Thiamine chloride hydrochlor...	11061401	1
Caelo	Thiamine chloride hydrochlor...	4071402	1
Caelo	Thiamine chloride hydrochlor...	12340712	1
Caelo	Thiamine chloride hydrochlor...	14069502	1
Caelo	Thiamine chloride hydrochlor...	12091407	1
Sanacorp	Thiamine chloride hydrochlor...	12340712	1
Fagron	Thiamine chloride hydrochlor...	13E22-No8	1
Fagron	Thiamine chloride hydrochlor...	10111401	1
Caelo	Thiamine chloride hydrochlor...	5122	1
Caelo	Thiamine chloride hydrochlor...	8121405	1
Caelo	Thiamine chloride hydrochlor...	13296610	4
Fagron	Thiamine chloride hydrochlor...	190115006	1
Caelo	Thiamine chloride hydrochlor...	15003201	1
Caelo	Thiamine chloride hydrochlor...	15199009	2
Caelo	Thiamine chloride hydrochlor...	15199099	1
Euro OTC	Thiamine chloride hydrochlor...	1705034-01	2
Caelo	Thiamine chloride hydrochlor...	16015607	1
Euro OTC	Thiamine chloride hydrochlor...	1712013-01	1
Euro OTC	Thiamine chloride hydrochlor...	1807001-01	1

- 78 896 spectra from 565 *Apo-Ident* customers from a total of 26 114 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Thiamine chloride hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Thiamine chloride hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	280	0	126 612
Type C	0	32	1	78 896

The substance/substance group *Thiamine chloride hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.8817 %)	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
21511	21511	0.00	40.76
21647	22477	6.46	40.76
22919	22919	0.00	34.97
22477	22477	0.00	47.18

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Thymol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20003-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Thymol; Thymolum

Special notes

When selecting the *Thymol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Thymol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Thymol	14025805	21469	40	20140127
Euro OTC	Thymol	1312022-02	21639	40	20131219
Euro OTC	Thymol	1510004	21943	40	20151016*

Validation samples

A total of 280 317 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 *Thymol*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 9 reference samples from the substance/substance group *Thymol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Thymol	14025805	21469 [†]	20
Euro OTC	Thymol	1312022-02	21639 [†]	20
Euro OTC	Thymol	1510004	21943 [†]	20
Caelo	Thymol	16144101	23160	40
Fagron	Thymol	15H13-B05-328912	23499	40
Euro OTC	Thymol	1710037	23773	40
Caelo	Thymol	173407	23837	40
Caelo	Thymol	181424	24231	40
Euro OTC	Thymol	1808014	24299	40

- 126 592 spectra from a total of 2780 batches from further 781 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*.

- 83 spectra from 68 *Apo-Ident* customers from 47 batches from the substance/substance group *Thymol*.

Supplier	Substance	Batch	Spectra
Caelo	Thymol	11358608	1
Fagron	Thymol	12E30-N11	1
Euro OTC	Thymol	20151012-1	1
Euro OTC	Thymol	1202028-01	1
Caelo	Thymol	11358607	2
Fagron	Thymol	12M29-N02	1
Fagron	Thymol	12H29-N02	2
Caelo	Thymol	11358616	1
Noweda	Thymol	12k01-no2	1
Fagron	Thymol	713575	1
Phönix	Thymol	11358610	1
Fagron	Thymol	12K01-N02	2
Sanacorp	Thymol	1135816	1
Caelo	Thymol	11178718	1
Caelo	Thymol	19061303	1
Caelo	Thymol	13147502	2
Caelo	Thymol	13288802	4
Sanacorp	Thymol	9E14-N16	1
Fagron	Thymol	12B06-N11	1
PHOENIX 26.03.2014	Thymol	14025802	2
Frey+Lau GmbH/Phönix	Thymol	1312022-01	1
Caesar § Lorenz GmbH	Thymol	13288806	1
Caelo	Thymol	14025802	2
	Thymol	14025802	1
Euro OTC	Thymol	1312022-01	1
Caelo	Thymol	14025809	2
ACM / Herba	Thymol	KNC1166J14	1
Caelo	Thymol	14025805	1
Gehe Kassel	Thymol	1312022-01	1
Caelo	Thymol	14025816	1
Caelo	Thymol	14025807	1
Caelo	Thymol	14310601	1
Euro OTC	Thymol	1410007-01	4
Caelo	Thymol	2031503	1
Caelo	Thymol	14310605	1
Caelo	Thymol	14302401	1
Caelo	Thymol	15130106	2
Caelo	Thymol	15130101	1
Euro OTC	Thymol	1510004-01	2
Caelo	Thymol	15362901	4
Caelo	Thymol	14025815	1
Ebert & Jacobi 02.08...	Thymol	15362901	1
Euro OTC	Thymol	1510004-02	6
Caelo	Thymol	15362908	2
Euro OTC	Thymol	11358603	1
Phönix	Thymol	1510004-01	1
Euro/ Phönix	Thymol	1510004-02	1
Caelo	Thymol	16144105	4
Euro OTC	Thymol	1510004-03	1
Noweda	Thymol	16144105	1
Caelo	Thymol	16144101	1
Caelo	Thymol	21042	1
Caelo	Thymol	17324203	1
Caelo	Thymol	16144108	1
Euro OTC	Thymol	1710037-01	2

- 78 846 spectra from 565 *Apo-Ident* customers from a total of 26 090 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Thymol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Thymol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	300	0	126 592
Type C	0	79	4	78 846

The substance/substance group *Thymol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.8817 %)	95.1807 % (> 91.5663 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21469	21943	17.67	55.69
21639	21943	25.75	54.21
21943	21943	0.00	62.61

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tobramycin sulfate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20951-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tobramycin sulfate; Tobramycin sulphate; Tobramycini sulfas

Special notes

When selecting the *Tobramycin sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tobramycin sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tobramycin sulfate	12G03-N03	20951	40	1404541
Euro OTC	Tobramycin sulfate	1301011-02	21624	40	1508071
Euro OTC	Tobramycin sulfate	1505015-01	21832	40	8963
Euro OTC	Tobramycin sulfate	1510035-01	22240	40	9202
Euro OTC	Tobramycin sulfate	1510035	22252	40	20151208*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tobramycin sulfate	15I17-B04-315697	22359	30	20150928
Audor	Tobramycin sulfate	AP15061047002T	22393	40	1608462
Fagron	Tobramycin sulfate	16B05-B03-336397	23515	40	1801385
Euro OTC	Tobramycin sulfate	1807045	24321	40	20180917*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 350 spectra of 9 reference samples from the substance/substance group *Tobramycin sulfate*. These samples are listed above in the [calibration samples](#) section.
- 74146 spectra from a total of 1614 batches from further 372 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 [†].

- 355 spectra of 10 reference samples from the substance/substance group *Tobramycin sulfate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tobramycin sulfate	1301011-02	21624 [†]	20
Euro OTC	Tobramycin sulfate	1505015-01	21832 [†]	20
Euro OTC	Tobramycin sulfate	1510035-01	22240 [†]	20
Euro OTC	Tobramycin sulfate	1510035	22252 [†]	20
Fagron	Tobramycin sulfate	15I17-B04-315697	22359 [†]	15
Audor Pharma	Tobramycin sulfate	AP15061047002T	23502	40
Euro OTC	Tobramycin sulfate	1710029	23870	40
Euro OTC	Tobramycin sulfate	1505015-01	21832SI	60
Euro OTC	Tobramycin sulfate	1510035-01	22240SI	60
Euro OTC	Tobramycin sulfate	1510035	22252SI	60

*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*.

- 126 537 spectra from a total of 2782 batches from further 781 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.

- 17 spectra from 7 *Apo-Ident* customers from 11 batches from the substance/substance group *Tobramycin sulfate*.

Supplier	Substance	Batch	Spectra
PHOENIX 31.01.2014	Tobramycin sulfate	1202006-01	1
Fagron	Tobramycin sulfate	15/17-B04-315697	1
Euro OTC	Tobramycin sulfate	1505015-01	1
Fagron	Tobramycin sulfate	13H09-N09	1
Euro OCT/Noweda	Tobramycin sulfate	1510035-01	1
Fagron	Tobramycin sulfate	16B05-B03-317988	2
Fagron	Tobramycin sulfate	16B05-B03	4
Euro OTC	Tobramycin sulfate	15I17-B04-315697	1
Fagron	Tobramycin sulfate	16B05-B03-319433	1
Fagron	Tobramycin sulfate	16B05-B03-330974	2
Fagron	Tobramycin sulfate	17E05-B03-338122	2

- 78 912 spectra from 565 *Apo-Ident* customers from a total of 26 126 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tobramycin sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tobramycin sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	350	0	74 146
Type B	0	271	84	126 537
Type C	0	15	2	78 912

The substance/substance group *Tobramycin sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.2857 %)
Type B	100.0000 % (> 99.9901 %)	76.3380 % (> 75.4930 %)
Type C	100.0000 % (> 99.8817 %)	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
22240	22240	0.00	37.71
22252	22252	0.00	23.63
21624	21624	0.00	15.73
20951	20951	0.00	17.72
21832	21832	0.00	20.41
22359	21832	11.61	21.83
23515	23515	0.00	17.82
22393	22393	0.00	17.45
24321	24321	0.00	36.00

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group	Tosylchloramide sodium
Substance class	APIs & excipients, solid
Report date	24/05/2019
Report number	20133-2019-05-24
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tosylchloramide sodium; Tosylchloramidum natricum

Special notes

When selecting the *Tosylchloramide sodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5	<i>European Pharmacopoeia 9th Edition, Basic Version 2017</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>
Appendix F	Addition to the second-stage models

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tosylchloramide sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tosylchloramide ...	13103201	20864	40	20130424
Caelo	Tosylchloramide ...	13361602	21115	40	1407634
Caelo	Tosylchloramide ...	16236603	23562	40	20160819

Validation samples

A total of 280 317 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 *Tosylchloramide sodium*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 3 reference samples from the substance/substance group *Tosylchloramide sodium*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tosylchloramide sodium	13361606	21480	60
Caelo	Tosylchloramide sodium	162366	22773	40
Caelo	Tosylchloramide sodium	172265	24238	40

- 126 752 spectra from a total of 2786 batches from further 781 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.

- 65 spectra from 37 *Apo-Ident* customers from 30 batches from the substance/substance group *Tosylchloramide sodium*.

Supplier	Substance	Batch	Spectra
Fagron	Tosylchloramide sodium	11L08-N04	1
Sanacorp	Tosylchloramide sodium	12H09-N01	1
Caelo	Tosylchloramide sodium	12277005	3
Anzag	Tosylchloramide sodium	12H09-N01	1

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Supplier	Substance	Batch	Spectra
Caelo	Tosylchloramide sodium	11116708	1
Caelo	Tosylchloramide sodium	12323605	1
Caelo	Tosylchloramide sodium	12323607	1
Caelo	Tosylchloramide sodium	12323606	1
Caelo	Tosylchloramide sodium	12323609	2
Caelo	Tosylchloramide sodium	72215377	2
Caelo	Tosylchloramide sodium	71051187	2
Caelo	Tosylchloramide sodium	13103207	1
Caelo	Tosylchloramide sodium	13103206	8
Caelo	Tosylchloramide sodium	13103210	2
Caelo	Tosylchloramide sodium	1310206	1
Fagron	Tosylchloramide sodium	14B27-B03-291967	1
Caelo	Tosylchloramide sodium	13361606	3
Caelo	Tosylchloramide sodium	13361607	6
Caelo	Tosylchloramide sodium	14183509	1
Caelo	Tosylchloramide sodium	15039603	4
Caelo	Tosylchloramide sodium	15183905	1
Caelo	Tosylchloramide sodium	15370501	3
Fagron	Tosylchloramide sodium	14L12-B01-301915	1
Caelo	Tosylchloramide sodium	15370505	1
Caelo	Tosylchloramide sodium	16236603	4
Caelo	Tosylchloramide sodium	16236607	5
Caelo	Tosylchloramide sodium	16236603/1180117	1
Caelo	Tosylchloramide sodium	17061503	2
Caeolo	Tosylchloramide sodium	16236607	1
Caelo	Tosylchloramide sodium	16236611	1
Caelo	Tosylchloramide sodium	17226503	1
EuRho	Tosylchloramide sodium	133610607	1

- 78 864 spectra from 565 *Apo-Ident* customers from a total of 26 108 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tosylchloramide sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tosylchloramide sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	139	1	126 752
Type C	0	55	10	78 864

The substance/substance group *Tosylchloramide sodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	99.2857 % (> 97.1429 %)
Type C	100.0000 % (> 99.8817 %)	84.6154 % (> 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
20864	21115	10.78	30.46
21115	21115	0.00	34.80
23562	21115	7.51	34.85

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tranexamic acid**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20397-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tranexamic acid; Acidum tranexamicum

Special notes

When selecting the *Tranexamic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tranexamic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tranexamic acid	14C21-B08-292225	21654	40	AR-17-FG-016394-01
Fagron	Tranexamic acid	14L15-B06-3000036	21727	40	AR-15-FG-008937-02
Fagron	Tranexamic acid	16E31-B07-331591	23505	40	20160622

Validation samples

A total of 280 317 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 *Tranexamic acid*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Tranexamic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Tranexamic acid	14C21-B08-292225	21654 [†]	20
Fagron	Tranexamic acid	14L15-B06-3000036	21727 [†]	20
Fagron	Tranexamic acid	16E31-B07-331591	23503	50
Audor Pharma	Tranexamic acid	APX1508016MT	23504	40

- 126 762 spectra from a total of 2785 batches from further 781 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.

- 21 spectra from 14 *Apo-Ident* customers from 17 batches from the substance/substance group *Tranexamic acid*.

Supplier	Substance	Batch	Spectra
Fagron	Tranexamic acid	12D11-N02	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	Tranexamic acid	13G24-N21	1
Fagron	Tranexamic acid	13D08-N24	1
Fagron	Tranexamic acid	13K08-B04-287966	1
Fagron	Tranexamic acid	13D08-N24	1
Fagron	Tranexamic acid	15J29-B04-312372	1
Fagron	Tranexamic acid	15J29-B04	1
Caelo	Tranexamic acid	15J29-B04	1
Fagron	Tranexamic acid	16J29-B04-312372	1
Audor Pharma	Tranexamic acid	1508016MT	1
Fagron	Tranexamic acid	16B03-B02-319617	2
Fagron	Tranexamic acid	13D08-N240002/40	1
Audor Pharma	Tranexamic acid	APX1508016MT	1
Audor Pharma	Tranexamic acid	APX1712011MT	3
Fagron	Tranexamic acid	18A17-B05-345038	1
Fagron	Tranexamic acid	5041804	1
Fagron	Tranexamic acid	18F20-B01-351693	1
Fagron	Tranexamic acid	18F20-B01-351691	1

- 78 908 spectra from 565 *Apo-Ident* customers from a total of 26 121 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tranexamic 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 *Tranexamic 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	120	0	74 376
Type B	0	130	0	126 762
Type C	0	19	2	78 908

The substance/substance group *Tranexamic 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 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.8817 %)	90.4762 % (> 76.1905 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21654	21654	0.00	77.62
21727	21727	0.00	83.65
23505	21654	3.26	78.33

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tretinoin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20474-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tretinoin; Tretinoinum

Special notes

When selecting the *Tretinoin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tretinoin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tretinoin	1402007-02	21747	40	1507085
Caelo	Tretinoin	15028403	21757	40	1507086
Caelo	Tretinoin	15239503	21878	20	20150717
Euro OTC	Tretinoin	1510007	21940	40	20151102*
Euro OTC	Tretinoin	1604059	22574	40	20160603*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tretinoin	15F01-B06-317884	22936	40	20150619
Euro OTC	Tretinoin	1402007-02	21747SI	40	1507085
Caelo	Tretinoin	15028403	21757SI	40	1507086
Caelo	Tretinoin	15239503	21878SI	40	20150717
Euro OTC	Tretinoin	1510007	21940SI	40	20151102*
Fagron	Tretinoin	15F01-B06-317884	22936SI	40	20150619

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 420 spectra of 11 reference samples from the substance/substance group *Tretinoin*. These samples are listed above in the [calibration samples](#) section.
- 74076 spectra from a total of 1617 batches from further 372 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 [†].

- 920 spectra of 27 reference samples from the substance/substance group *Tretinoin*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tretinoin	1402007-02	21747 [†]	20
Caelo	Tretinoin	15028403	21757 [†]	20
Caelo	Tretinoin	15239503	21878 [†]	40
Euro OTC	Tretinoin	1510007	21940 [†]	20
Caelo	Tretinoin	162915	22779	40
Caelo	Tretinoin	162171	22780	40
Euro OTC	Tretinoin	1612010	22911	40
Caelo	Tretinoin	172731	23680	40
Caelo	Tretinoin	173057	23843	40
Euro OTC	Tretinoin	1804005	24061	40
Caelo	Tretinoin	181673	24251	40
Caelo	Tretinoin	181674	24258	40
Euro OTC	Tretinoin	1901001	24456	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
Euro OTC	Tretinoin	1402007-02	21747SI [†]	20
Caelo	Tretinoin	15028403	21757SI [†]	20
Caelo	Tretinoin	15239503	21878SI [†]	20
Euro OTC	Tretinoin	1510007	21940SI [†]	20
Euro OTC	Tretinoin	1604059	22574SI	40
Caelo	Tretinoin	162915	22779SI	40
Caelo	Tretinoin	162171	22780SI	40
Euro OTC	Tretinoin	1612010	22911SI	40
Caelo	Tretinoin	172731	23680SI	40
Caelo	Tretinoin	173057	23843SI	40
Euro OTC	Tretinoin	1804005	24061SI	40
Caelo	Tretinoin	181673	24251SI	20
Caelo	Tretinoin	181674	24258SI	40
Euro OTC	Tretinoin	1901001	24456SI	40

- 125 972 spectra from a total of 2775 batches from further 781 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.

- 481 spectra from 232 *Apo-Ident* customers from 178 batches from the substance/substance group *Tretinoin*.

Supplier	Substance	Batch	Spectra
Caelo	Tretinoin	12023302	9
Caelo	Tretinoin	12102902	1
Noweda	Tretinoin	12023302	2
Caelo	Tretinoin	12102904	2
Caelo	Tretinoin	11225506	1
Caelo	Tretinoin	11284703	1
Caelo	Tretinoin	11225504	1
Euro OTC	Tretinoin	1109014-02	2
Caesar & Loretz GmbH	Tretinoin	11225515	1
Phönix	Tretinoin	1109014-02	1
Caelo	Tretinoin	711212563	1
Caelo	Tretinoin	11225511	1
Caesar & Loretz GmbH, 4...	Tretinoin	12023302	1
Caelo	Tretinoin	1109014-02	1
Caelo	Tretinoin	5012I-02563	1
Fagron	Tretinoin	12106-N01	1
Caelo	Tretinoin	12106-N01	1
Caelo	Tretinoin	12320201	2
Caelo	Tretinoin	12D05-N08	1
Fagron	Tretinoin	11K29-N01	1
Sanacorp	Tretinoin	12320302	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	Tretinoin	12023309	1
Caelo	Tretinoin	12320205	5
Caelo	Tretinoin	3041302	1
Caelo	Tretinoin	12320204	1
Caelo	Tretinoin	12320301	1
Caelo	Tretinoin	12102903	2
Caelo	Tretinoin	12320203	2
Caelo	Tretinoin	12320207	1
Caelo	Tretinoin	12367103	2
Caelo	Tretinoin	12320209	6
Euro OTC	Tretinoin	1008021-02	1
Fagron	Tretinoin	12I06-N01	2
Caelo	Tretinoin	12320303	1
Caelo	Tretinoin	12367101	2
Caelo	Tretinoin	12023303	1
Phoenix	Tretinoin	12367103	1
Euro OTC	Tretinoin	10429AX21	1
Euro OTC	Tretinoin	13041028-01	1
Euro OTC	Tretinoin	1304028-01	7
Fagron	Tretinoin	20120601	1
Noweda	Tretinoin	13D30-N14	1
Caelo	Tretinoin	12367104	1
Caelo	Tretinoin	20120601	1
Sanacorp	Tretinoin	12/06-N01	1
Fagron	Tretinoin	13D30-N14	2
Caesar & Loretz GmbH	Tretinoin	12320211	1
Fagron	Tretinoin	13D30-N14-3365319091	1
Caelo	Tretinoin	13278101	1
Caelo	Tretinoin	13195002	14
Caelo	Tretinoin	13278104	2
Caelo	Tretinoin	13278102	4
BASF/Phönix	Tretinoin	1304028-02	2
Caelo	Tretinoin	1304028-02	2
Fagron	Tretinoin	13B05-B02-287360	4
Caelo	Tretinoin	13278105	2
Euro OTC	Tretinoin	130402802	1
Fagron	Tretinoin	13B05-B02-287361	2
cealo	Tretinoin	13195002	1
Caelo	Tretinoin	131950002	1
Fagron	Tretinoin	13C11-N06	2
Caelo	Tretinoin	13195008	1
Caelo	Tretinoin	13308003	1
Euro OTC	Tretinoin	1304028-02	4
Caelo	Tretinoin	13308004	4
EuRho/Sanacorp	Tretinoin	130402802	1
Caelo	Tretinoin	14093502	4
Fagron	Tretinoin	13D30N14	1
Caelo	Tretinoin	13B05-B02-287360	1
Sanacorp	Tretinoin	13308004	1
Euro OTC	Tretinoin	30042014A	1
Caelo	Tretinoin	14040504	5
Euro OTC	Tretinoin	130102802	1
Caelo	Tretinoin	14093503	1
Fagron	Tretinoin	14093505	1
Euro OTC	Tretinoin	1402007-01	5
Euro OTC	Tretinoin	140200701	1
Phönix	Tretinoin	14D09-B04	2
Phönix	Tretinoin	14D09-B04-293224	1
Euro OTC	Tretinoin	1402007-02	8
Fagron	Tretinoin	14D09-B04-293225	1

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Supplier	Substance	Batch	Spectra
Fagron	Tretinoin	14040504	1
Fagron	Tretinoin	14D09-B04-293224	1
Euro OTC	Tretinoin	1402007	1
Fagron	Tretinoin	14D09-B04-293594	1
Euro OTC	Tretinoin	140200703	1
Fargron	Tretinoin	14D09-B04-293225	1
Bombastus	Tretinoin	1402007-03	1
Euro OTC	Tretinoin	1402007-03	3
Caelo	Tretinoin	14040507	1
Caelo	Tretinoin	14252801	1
Caelo	Tretinoin	14252702	3
BASF	Tretinoin	1402007-03	1
Phönix	Tretinoin	1402007-02	1
Caelo	Tretinoin	1452802	1
Fargron	Tretinoin	1402007-01	1
Caelo	Tretinoin	14252710	2
Fagron	Tretinoin	14D09-B04-295551	1
Sanacorp	Tretinoin	1411016-01	1
Euro OTC	Tretinoin	1411016-01	9
Caelo	Tretinoin	14252706	2
Fagron	Tretinoin	1440104	1
Euro OTC	Tretinoin	14020007-01	1
Euro	Tretinoin	14111016-01	1
Fagron	Tretinoin	14L24-B01	1
Caelo	Tretinoin	1411016-01	1
Fagron	Tretinoin	14L24-B01-303152	1
Caelo	Tretinoin	15078302	2
Sanacorp	Tretinoin	1411016-02	1
Fagron	Tretinoin	1410001594	1
Euro OTC	Tretinoin	141101602	1
Fagron	Tretinoin	14L24-B01-303157	3
Caelo	Tretinoin	15239501	2
Fagron	Tretinoin	1411016-01	1
Caelo	Tretinoin	15078303	1
Caelo	Tretinoin	15239503	2
Euro OTC	Tretinoin	1411016-02	11
Anzag/Henry Lamotte	Tretinoin	15078303	1
Euro OTC	Tretinoin	141107602	1
Caelo	Tretinoin	15239502	5
Euro OTC	Tretinoin	14101602	1
Fagron	Tretinoin	15F01-B06-308856	2
Fagron	Tretinoin	15F01-B06-308722	5
Caelo	Tretinoin	14L24-B01-303157	2
Anzag	Tretinoin	15078305	1
Noweda	Tretinoin	15078307	1
Eurimpharm	Tretinoin	1411016-01	1
Nachprüfung	Tretinoin		1
Caelo	Tretinoin	15078308	1
Caelo	Tretinoin	15078307	3
Euro OTC	Tretinoin	151000	1
Euro OTC	Tretinoin	1510007-01	9
Caelo	Tretinoin	15078305	2
Euro OTC	Tretinoin	140007-02	1
Euro OTC	Tretinoin	1510007-02	8
Caelo	Tretinoin	151000701	1
Noweda	Tretinoin	15F01-B06-315491	1
Caelo	Tretinoin	16070002	2
EuRho	Tretinoin	151007-01	1
Fagron	Tretinoin	1510007-02	1
Caelo	Tretinoin	1510007-02	1

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Supplier	Substance	Batch	Spectra
Caelo	Tretinoin	15078301	1
Caelo	Tretinoin	16070001	1
Fagron	Tretinoin	14009-804	1
Caelo	Tretinoin	15437301	1
Euro OTC	Tretinoin	1604059-01	16
Fagron	Tretinoin	15F01-B06-315491	1
Caelo	Tretinoin	15F01-B06-308856	1
WE:Phönix 20.08.2016 E...	Tretinoin	1510007-02	1
Fagron	Tretinoin	15F01-B06-317884	1
Euro OTC	Tretinoin	12959AX20	2
Euro OCT Pharma/Fiebig	Tretinoin	1604059-01	2
Caelo	Tretinoin	15H31-B01	1
Phoenix	Tretinoin	15F01-B06-317884	1
Caelo	Tretinoin	15437303	8
Fagron	Tretinoin	231115T	1
WE:Phönix 02.11..2016 ...	Tretinoin	1604059-01	1
Euro OTC	Tretinoin	165070002	1
Fagron	Tretinoin	16F14-B04	3
Celo	Tretinoin	15437303	1
Fagron	Tretinoin	1604059-01	1
Euro/Gehe	Tretinoin	1604059-01	1
Euro OTC	Tretinoin	160405902	1
Caelo	Tretinoin	16F14-B04	1
Euro OTC	Tretinoin	1604059-02	13
Gehe	Tretinoin	15437303	1
Caelo	Tretinoin	16291503	4
Caelo	Tretinoin	16F14-B04-324636	1
Caelo	Tretinoin	16291502	4
Fagron	Tretinoin	16F14-B04-325560	2
Fagron	Tretinoin	16F14B04325560	1
Caelo	Tretinoin	160405901	1
Caelo	Tretinoin	1612010-01	3
Euro OTC	Tretinoin	16004059-02	1
Caelo	Tretinoin	1517E-02563	1
Euro OTC	Tretinoin	1612010-01	16
Caelo	Tretinoin	16217107	1
Fagron	Tretinoin	16F14-B04-326181	2
Gatt-Koller	Tretinoin	606210909	1
Caelo	Tretinoin	17106102	5
Caelo	Tretinoin	17106101	5
Fagron	Tretinoin	16K03-B06-328388	4
Euro/Noweda	Tretinoin	1612010-01	1
Gehe	Tretinoin	1612010-01	1
Euro OTC	Tretinoin	161210-01	1
Caelo	Tretinoin	16F14-B04-326181	1
Fagron	Tretinoin	16F14-B04-325567	1
Caelo	Tretinoin	16217108	3
Fagron	Tretinoin	16K03-B06	2
Fagron	Tretinoin	170706TTRER-20151004	1
Euro/Sanacorp	Tretinoin	1604059-02	1
Caelo	Tretinoin	16K03-806328-388	1
Caelo	Tretinoin	171061025343	1
phönix	Tretinoin	1612010-01	1
Euro OTC	Tretinoin	1612010-02	7
Krieger	Tretinoin	1612010-02	2
Sanacorp	Tretinoin	16217122	1
Fargon	Tretinoin	16K03-B06-328388	1
Euro OTC	Tretinoin	161201001	1
Gehe-Eurho 22.11.2017	Tretinoin	2171127Ma7	1
Caelo	Tretinoin	1604059-02	1

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Supplier	Substance	Batch	Spectra
Caelo	Tretinoin	172773102	1
Caelo	Tretinoin	17305702	3
Caelo	Tretinoin	17305701	4
Phönix WE:04.01.18 E.K. ...	Tretinoin	17273102	1
Fagron	Tretinoin	17273102	1
Fagron	Tretinoin	17K01-B05-341936	2
Caelo	Tretinoin	17357001	2
Caelo	Tretinoin	17305707	3
Caelo	Tretinoin	17305704	1
Fagron	Tretinoin	17K01-B05-341941	1
Caelo	Tretinoin	1735707	1
Caelo	Tretinoin	173057075597	1
Sanacorp	Tretinoin	17357001	1
Caelo	Tretinoin	17357005	2
Euro OTC	Tretinoin	1804005-01	7
Fagron	Tretinoin	17357007	1
Caelo	Tretinoin	17305708	1
Caelo	Tretinoin	17305711	1
Caelo	Tretinoin	17357008	3
Kehr	Tretinoin	1604059-01	1
Fagron	Tretinoin	17K01-B05-345784	2
Caelo	Tretinoin	17357007	2
Caelo	Tretinoin	17305710	1
Caelo	Tretinoin	17357002	1
Caelo	Tretinoin	18167401	1
Apo Ident/ Noweda	Tretinoin	1804005-01	1
Fagron	Tretinoin	17K01-B05-347435	1
Fagron	Tretinoin	17K01-B05-347436	1
Fagron	Tretinoin	17K01-B05	1
Caelo	Tretinoin	18167301	1
Sanacorp	Tretinoin	1804005-01	1
Fagron	Tretinoin	17K01B05349946	1
Euro OTC	Tretinoin	18062082	1
Caelo	Tretinoin	18167309	1
Caelo	Tretinoin	18167410	1

- 78 448 spectra from 565 *Apo-Ident* customers from a total of 25 962 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tretinoin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tretinoin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	74 076
Type B	0	918	2	125 972
Type C	0	367	114	78 448

The substance/substance group *Tretinoin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9901 %)	99.7826 % (> 99.4565 %)
Type C	100.0000 % (> 99.8817 %)	76.2994 % (> 75.6757 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
22936	21940	2.42	43.99
21747	21747	0.00	48.41
21940	21940	0.00	44.57
21757	21757	0.00	41.75
22574	22574	0.00	44.23
21878	21747	12.41	47.06

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Triamcinolone acetonide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20765-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Triamcinolone acetonide; Triamcinoloni acetamidum

Special notes

When selecting the *Triamcinolone acetonide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Triamcinolone acetonide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Triamcinolone ac...	12E15-N03	20765	50	1412051
Euro OTC	Triamcinolone ac...	1303001-02	20910	40	20130815
Caelo	Triamcinolone ac...	13256607	21061	100	AR-15-FG-003755-01
Euro OTC	Triamcinolone ac...	1211013-02	21072	30	20130417
Caelo	Triamcinolone ac...	13379921	21587	40	1503634

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Triamcinolone ac...	1508008	21883	40	20150902*
Fagron	Triamcinolone ac...	15C19-B06-308572	21962	40	20150402
Euro OTC	Triamcinolone ac...	1601021	22313	30	20160119*
Euro OTC	Triamcinolone ac...	1605010	22572	40	20160531*
Euro OTC	Triamcinolone ac...	1608005	22752	40	20160906*
Euro OTC	Triamcinolone ac...	1605010	22572SI	25	20160531*
Euro OTC	Triamcinolone ac...	1608005	22752SI	22	20160906*

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 497 spectra of 12 reference samples from the substance/substance group *Triamcinolone acetone*. These samples are listed above in the [calibration samples](#) section.
- 73999 spectra from a total of 1613 batches from further 372 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 [†].

- 963 spectra of 31 reference samples from the substance/substance group *Triamcinolone acetone*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Triamcinolone acetone	12E15-N03	20765 [†]	10
Caelo	Triamcinolone acetone	12301505	20769	60
Fagron	Triamcinolone acetone	13C13-N20	21043	60
Caelo	Triamcinolone acetone	13379921	21587 [†]	20
Euro OTC	Triamcinolone acetone	1508008	21883 [†]	20
Fagron	Triamcinolone acetone	15C19-B06-308572	21962 [†]	20
Euro OTC	Triamcinolone acetone	1601021	22313 [†]	15
Caelo	Triamcinolone acetone	160945	22473	60
Euro OTC	Triamcinolone acetone	1612014	22978	40
Caelo	Triamcinolone acetone	171206	23330	40
Caelo	Triamcinolone acetone	171206	23343	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
Euro OTC	Triamcinolone acetonide	1703037	23393	40
Euro OTC	Triamcinolone acetonide	1706013	23557	40
Euro OTC	Triamcinolone acetonide	1710002	23694	40
Euro OTC	Triamcinolone acetonide	1801020	23883	40
Caelo	Triamcinolone acetonide	181002	24016	40
Euro OTC	Triamcinolone acetonide	1805001-01	24191	40
Euro OTC	Triamcinolone acetonide	1810015	24333	40
Euro OTC	Triamcinolone acetonide	1508008	21883SI	30
Fagron	Triamcinolone acetonide	15C19-B06-308572	21962SI	19
Caelo	Triamcinolone acetonide	160945	22473SI	40
Euro OTC	Triamcinolone acetonide	1612014	22978SI	29
Caelo	Triamcinolone acetonide	171206	23330SI	20
Caelo	Triamcinolone acetonide	171206	23343SI	20
Euro OTC	Triamcinolone acetonide	1703037	23393SI	20
Euro OTC	Triamcinolone acetonide	1706013	23557SI	20
Euro OTC	Triamcinolone acetonide	1710002	23694SI	20
Euro OTC	Triamcinolone acetonide	1801020	23883SI	20
Caelo	Triamcinolone acetonide	181002	24016SI	20
Euro OTC	Triamcinolone acetonide	1805001-01	24191SI	20
Euro OTC	Triamcinolone acetonide	1810015	24333SI	20

- 125 929 spectra from a total of 2772 batches from further 781 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.

- 1632 spectra from 430 *Apo-Ident* customers from 375 batches from the substance/substance group *Triamcinolone acetonide*.

Supplier	Substance	Batch	Spectra
Euro OTC	Triamcinolone acetonide	1110005-01	1
Fagron	Triamcinolone acetonide	11K11-N10	5
Fagron	Triamcinolone acetonide	11N11-N10	1
Caelo	Triamcinolone acetonide	11267704	1
Fagron	Triamcinolone acetonide	5061205	1
Fagron	Triamcinolone acetonide	12B08-N01	7
Euro OTC	Triamcinolone acetonide	1112023-01	1
Caelo	Triamcinolone acetonide	10220341	1
Fagron	Triamcinolone acetonide	C22H25CIN209	1
Caelo	Triamcinolone acetonide	1107212516	1
Gehe	Triamcinolone acetonide	700124-0007	1
Fagron	Triamcinolone acetonide	12E15-N03	21
Euro OTC	Triamcinolone acetonide	1112023-02	3
Caelo	Triamcinolone acetonide	11267710	2
Caelo	Triamcinolone acetonide	NS0571M	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
Caesar&loretz,Phoenix	Triamcinolone acetonide	11267705	1
Caelo	Triamcinolone acetonide	1110005-01	1
Fagron	Triamcinolone acetonide	11B22-N05	1
Euro OTC	Triamcinolone acetonide	1206008-01	4
Caelo	Triamcinolone acetonide	11267721	2
Caelo	Triamcinolone acetonide	12173701	5
Caelo	Triamcinolone acetonide	11267707	4
Europharm/Sanacorp	Triamcinolone acetonide	B0544/111040	2
Europharm/Otto	Triamcinolone acetonide	1206008-01	1
Euro OTC	Triamcinolone acetonide	1209040-01	3
Caelo	Triamcinolone acetonide	12173705	2
Fagron	Triamcinolone acetonide	NS0571M	5
Noweda	Triamcinolone acetonide	1112023-02	1
Fagron	Triamcinolone acetonide	NS0571M	1
Fagron	Triamcinolone acetonide	13121201	1
Caelo	Triamcinolone acetonide	11267720	1
Caelo	Triamcinolone acetonide	1209040-01	1
Euro OTC	Triamcinolone acetonide	B0544/111404	1
Euro OTC	Triamcinolone acetonide	20130912-5	1
Caelo	Triamcinolone acetonide	12173707	5
Caelo	Triamcinolone acetonide	12173710	4
Noweda	Triamcinolone acetonide	12E15-N03	1
Caelo	Triamcinolone acetonide	9364429	2
Euro OTC	Triamcinolone acetonide	1209040-02	2
Fagron	Triamcinolone acetonide	1210-N09	1
Fagron	Triamcinolone acetonide	12I10-N09	4
Euro OTC	Triamcinolone acetonide	1211013-01	4
Fagron	Triamcinolone acetonide	12110-N09	3
Noweda	Triamcinolone acetonide	12301501	1
Gehe	Triamcinolone acetonide	12E15-N03	1
Caelo	Triamcinolone acetonide	12301501	4
Euro OTC	Triamcinolone acetonide	1013I-02516	1
Fagron	Triamcinolone acetonide	12/10-N09	3
Caelo	Triamcinolone acetonide	12173704	2
Fagron	Triamcinolone acetonide	120600801	1
Caesar&loretz,Phoenix	Triamcinolone acetonide	12173703	1
Fagron	Triamcinolone acetonide	20031302	1
Fagron	Triamcinolone acetonide	NS0996M	2
Gehe	Triamcinolone acetonide	12/10-N09	1
Caelo	Triamcinolone acetonide	12301506	1
Caelo	Triamcinolone acetonide	12/10-N09	3
Caesar&loretz,Phoenix	Triamcinolone acetonide	12301502	1
Europharm/Otto	Triamcinolone acetonide	1209040-02	1
Fagron	Triamcinolone acetonide	9041305	1
Sanacorp	Triamcinolone acetonide	12301506	1
Caelo	Triamcinolone acetonide	12301508	4
Caelo	Triamcinolone acetonide	120904002	1
Fagron	Triamcinolone acetonide	3212U-02516(NP)	1
Caelo	Triamcinolone acetonide	12301503	1
Caelo	Triamcinolone acetonide	12301504	1
Euro OTC	Triamcinolone acetonide	111005-01	1
Caelo	Triamcinolone acetonide	12301509	4
Europharm/Sanacorp	Triamcinolone acetonide	1211013-01	3
Hirsch	Triamcinolone acetonide	12I10-N09	2
Caelo	Triamcinolone acetonide	93/AD1	1
Fagron	Triamcinolone acetonide	13C13-20	1
Caelo	Triamcinolone acetonide	1201506	1
Euro OTC	Triamcinolone acetonide	1211013-02	9
Caelo	Triamcinolone acetonide	11267705	1
Noweda/ NEWCHEM	Triamcinolone acetonide	1211013-02	1

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Supplier	Substance	Batch	Spectra
Noweda	Triamcinolone acetonide	12301509	1
Caelo	Triamcinolone acetonide	12301515	11
Fagron	Triamcinolone acetonide		1
Fagron	Triamcinolone acetonide	5061303	1
Gehe	Triamcinolone acetonide	12301510	2
fargon	Triamcinolone acetonide	13C13-N20	1
Caelo	Triamcinolone acetonide	2513M02516	1
Caelo	Triamcinolone acetonide	12301510	4
Euro OTC	Triamcinolone acetonide	12G6008-01	1
Caelo	Triamcinolone acetonide	12301507	4
Fagron	Triamcinolone acetonide	13c13-n20	1
Fagron	Triamcinolone acetonide	13C13-N20	13
Apotheke Mildenau	Triamcinolone acetonide	13C13-N20	1
Caelo	Triamcinolone acetonide	12301518	4
Caelo	Triamcinolone acetonide	13E15-N03	1
Caelo	Triamcinolone acetonide	13C13-N20	2
Caelo	Triamcinolone acetonide	9081305	1
Euro OTC	Triamcinolone acetonide	121113-02	1
Alliance Healthcare	Triamcinolone acetonide	13C13-N20	1
Fagron	Triamcinolone acetonide	13E15-N03	41
Caelo	Triamcinolone acetonide	13124804	11
cesar&lorentz/Phönix	Triamcinolone acetonide	13124801	2
Caelo	Triamcinolone acetonide	13124806	2
Fagron	Triamcinolone acetonide	13E15N03	3
Noveda	Triamcinolone acetonide	12301518	1
Caelo	Triamcinolone acetonide	13e15-n03	2
Caelo	Triamcinolone acetonide	13124801	5
Gehe	Triamcinolone acetonide	13124805	1
Euro OTC	Triamcinolone acetonide	1303001-02	8
Euro OTC	Triamcinolone acetonide	13030001-01	1
Caelo	Triamcinolone acetonide	1210-n09	1
euro	Triamcinolone acetonide	1211013-02	1
Caelo	Triamcinolone acetonide	13124803	2
Caelo	Triamcinolone acetonide	4613E2516	1
Caelo	Triamcinolone acetonide	1811211	1
Euro OTC	Triamcinolone acetonide	1303001-01	1
Caelo	Triamcinolone acetonide	13124805	7
Euro OTC	Triamcinolone acetonide	1307043-01	14
Fagron	Triamcinolone acetonide	12B08N01	1
Anzag	Triamcinolone acetonide	1303001-02	1
Phönix	Triamcinolone acetonide	12E15-N03	1
Caelo	Triamcinolone acetonide	13256607	5
Sanacorp	Triamcinolone acetonide	13124807	2
Caelo	Triamcinolone acetonide	13124810	1
Caelo	Triamcinolone acetonide	1312407	1
Euro	Triamcinolone acetonide	1303001-02	1
Euro OTC	Triamcinolone acetonide	PT49	1
Caelo	Triamcinolone acetonide	13124807	11
Caelo	Triamcinolone acetonide	13124809	1
Fagron	Triamcinolone acetonide	411082-1-P	1
Caelo	Triamcinolone acetonide	95/AKD34	1
Caelo	Triamcinolone acetonide	3041206	1
Sanacorp	Triamcinolone acetonide	13E15-N03	1
Fagron	Triamcinolone acetonide	12301503	1
Caelo	Triamcinolone acetonide	13124808	13
EuRho/Phönix	Triamcinolone acetonide	1211013-01	1
Newchem	Triamcinolone acetonide	1303001-02	1
Euro OTC	Triamcinolone acetonide	1307043-02	13
Caelo	Triamcinolone acetonide	1206008-01	1
Caelo	Triamcinolone acetonide	13124811	4

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Supplier	Substance	Batch	Spectra
Fargon/Anzag	Triamcinolone acetonide	13/26-N11	3
Fargon	Triamcinolone acetonide	13I26-N11	11
Caelo	Triamcinolone acetonide	13379903	1
noweda	Triamcinolone acetonide	13256604	1
Fargon	Triamcinolone acetonide	13K15-B31-289025	1
Caelo	Triamcinolone acetonide	13256604	6
Caelo	Triamcinolone acetonide	1514Q2516	1
Gehe	Triamcinolone acetonide	13I26-N11	1
Euro OTC	Triamcinolone acetonide	15042014A	1
VDL	Triamcinolone acetonide	13379903	1
Phönix	Triamcinolone acetonide	13379902	1
Sanacorp	Triamcinolone acetonide	1326N11	1
Fargon	Triamcinolone acetonide	NT0487M	1
Caelo	Triamcinolone acetonide	6051401	1
euroct/gehe	Triamcinolone acetonide	1403009	1
EuRho/Phönix	Triamcinolone acetonide	1307043-02	1
Fargon	Triamcinolone acetonide	13/26-N11	6
Caelo	Triamcinolone acetonide	13379913	4
Caelo	Triamcinolone acetonide	13I26-N11	1
Fargon	Triamcinolone acetonide	13K15-B31	5
Caelo	Triamcinolone acetonide	13256608	2
Noweda	Triamcinolone acetonide	13K15-B31-289029	1
Fargon	Triamcinolone acetonide	NT077oM	1
Euro OTC	Triamcinolone acetonide	1403009-01	3
Fargon	Triamcinolone acetonide	13K15B31289029	1
Fargon	Triamcinolone acetonide	1326-N11	1
	Triamcinolone acetonide	1403009-01	1
Fargon	Triamcinolone acetonide	13K15-B31-289029	3
Fargon	Triamcinolone acetonide	13126-N11	1
Fargon	Triamcinolone acetonide	13K15-B31-289031	4
Euro OTC	Triamcinolone acetonide	14030009-01	2
Caelo	Triamcinolone acetonide	13379904	4
Euro OTC	Triamcinolone acetonide	1403009-02	12
Caelo	Triamcinolone acetonide	13379914	4
Martinus-Apotheke	Triamcinolone acetonide	13379905	1
Fargon	Triamcinolone acetonide	NT0770M	1
Phönix	Triamcinolone acetonide	1403009-01	1
Fargon	Triamcinolone acetonide	NT1094M	1
Caelo	Triamcinolone acetonide	13379905	13
Caelo	Triamcinolone acetonide	13256603	1
Apomix/Phönix	Triamcinolone acetonide	13k15-b31-289029	2
Caelo	Triamcinolone acetonide	13379906	5
euroct/gehe	Triamcinolone acetonide	1403009-02	1
EuRho	Triamcinolone acetonide	1403009-02	1
Fargon	Triamcinolone acetonide	13/26-N11	1
Euro OTC	Triamcinolone acetonide	14030009-02	1
Sanacorp	Triamcinolone acetonide	13379905	1
Caelo	Triamcinolone acetonide	13K15-B31-289029	1
Caelo	Triamcinolone acetonide	13379912	8
Caelo	Triamcinolone acetonide	13K15-B31-289027	2
Fargon	Triamcinolone acetonide	13K14-B04	2
Euro OTC	Triamcinolone acetonide	1407044-01	7
Fargon	Triamcinolone acetonide	13K15-B31-289027	3
Phoenix	Triamcinolone acetonide	13126-N11	2
Newchem/ Noweda	Triamcinolone acetonide	1403009-01	1
Phönix	Triamcinolone acetonide	13K15-B31-289027	1
Caelo	Triamcinolone acetonide	14188302	5
Caelo	Triamcinolone acetonide	13379901	1
Caelo	Triamcinolone acetonide	13379911	1
Fargon	Triamcinolone acetonide	NT1430M	3

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Supplier	Substance	Batch	Spectra
Caelo	Triamcinolone acetonide	14188304	2
Euro OTC	Triamcinolone acetonide	14188304	1
EuRho/Phönix	Triamcinolone acetonide	1407044-01	1
Fagron	Triamcinolone acetonide	13K14-B04-289032	4
Newchem/Kehr	Triamcinolone acetonide	1407044-01	1
Fagron	Triamcinolone acetonide	14F30-B01-296287	3
Fagron	Triamcinolone acetonide	13k15-b31-289030	1
Euro OTC	Triamcinolone acetonide	1407044-02	13
Fagron	Triamcinolone acetonide	13K14-B04-289033	10
Caesar & Loretz GmbH Hi...	Triamcinolone acetonide	13379905	1
Phönix	Triamcinolone acetonide	1407044-01	1
Caelo	Triamcinolone acetonide	13379919	1
Caelo	Triamcinolone acetonide	14355103	11
Euro OTC	Triamcinolone acetonide	3022015A	1
Caelo	Triamcinolone acetonide	13379921	1
Fagron	Triamcinolone acetonide	13k14-B04-289032	1
Euro OTC	Triamcinolone acetonide	1412013-01	12
Caelo	Triamcinolone acetonide	14188303	3
AHD 03.03.2015	Triamcinolone acetonide	NT1430M	1
Anzag	Triamcinolone acetonide	14355103	1
Caelo	Triamcinolone acetonide	14355101	9
Fagron	Triamcinolone acetonide	1407044-01	1
Newchem/AHD	Triamcinolone acetonide	1407044-02	1
AHD 06.03.15 9,47	Triamcinolone acetonide	14355102	2
Caelo	Triamcinolone acetonide	13379922	1
Fagron	Triamcinolone acetonide	14F30-B01	1
Caelo	Triamcinolone acetonide	14355104	2
Caelo	Triamcinolone acetonide	12301505	1
Noweda	Triamcinolone acetonide	1407044-01	1
Caelo	Triamcinolone acetonide	12301502	1
Caelo	Triamcinolone acetonide	13K15-B31-289031	1
Euro OTC	Triamcinolone acetonide	1412013-02	6
Caelo	Triamcinolone acetonide	14355102	13
Fagron	Triamcinolone acetonide	13i26-N11	1
Berkel AHK	Triamcinolone acetonide	14355101	3
Euro OTC	Triamcinolone acetonide	141201301	1
Caelo	Triamcinolone acetonide	13K14-B04-289033	1
Fagron	Triamcinolone acetonide	NU0930M	1
Caelo	Triamcinolone acetonide	14355708	8
Euro OTC	Triamcinolone acetonide	141201302	3
Fagron	Triamcinolone acetonide	14355104	1
Fagron	Triamcinolone acetonide	14G23-B07-297619	1
Euro OTC	Triamcinolone acetonide	141213-02	1
Euro OTC	Triamcinolone acetonide	1504007-01	9
Fagron	Triamcinolone acetonide	14G23-B07-297620	3
Fagron	Triamcinolone acetonide	14G23-B07-297620	1
Caelo	Triamcinolone acetonide	1355101	1
Caelo	Triamcinolone acetonide	14355702	11
Fagron	Triamcinolone acetonide	14G23-B07-297618	3
Caelo	Triamcinolone acetonide	14G23-B07-297619	1
Fagron	Triamcinolone acetonide	1412013-01	1
Fagron	Triamcinolone acetonide	14K24N-N01	1
Caelo	Triamcinolone acetonide	14355711	6
Fagron	Triamcinolone acetonide	15B02-B03	4
Caelo	Triamcinolone acetonide	14355703	3
Caelo	Triamcinolone acetonide	14355704	2
Fargon/Alliance HC	Triamcinolone acetonide	15B02-B03-303830	1
Euro OTC	Triamcinolone acetonide	150400701	2
Phoenix	Triamcinolone acetonide	14355708	1
Fagron	Triamcinolone acetonide	15B02-B03-303830	7

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Supplier	Substance	Batch	Spectra
euro/ Anzag	Triamcinolone acetonide	3315I02516	1
Euro OTC	Triamcinolone acetonide	14120130	1
Eigen/Defektur	Triamcinolone acetonide	U0544/113530	1
Euro OTC	Triamcinolone acetonide	1504007-02	14
Fagron	Triamcinolone acetonide	14K14-B05-302887	1
Noweda	Triamcinolone acetonide	14355708	1
Noweda	Triamcinolone acetonide	14355103	1
Caelo	Triamcinolone acetonide	15233901	8
Caelo	Triamcinolone acetonide	15233902	17
Anzag	Triamcinolone acetonide	14355711	1
Farmabios S.p.A./Caesar...	Triamcinolone acetonide	15233901	1
Euro OTC	Triamcinolone acetonide	15404007-01	1
Caelo	Triamcinolone acetonide	15C19-B06-308573	1
Fagron	Triamcinolone acetonide	Nw0635M	1
Caelo	Triamcinolone acetonide	1508008-01	2
Euro OTC	Triamcinolone acetonide	NV0635M	1
Fagron	Triamcinolone acetonide	15C19-B06-308572	5
Caelo	Triamcinolone acetonide	15233905	6
Euro OTC	Triamcinolone acetonide	1508008-01	12
AHD/Hedinger	Triamcinolone acetonide	15233902	1
Fagron	Triamcinolone acetonide	15C19-B06-308571	1
Fagron	Triamcinolone acetonide	NV0262M	1
Fargon	Triamcinolone acetonide	Nu2526M	1
Fagron	Triamcinolone acetonide	14355709	1
Caelo	Triamcinolone acetonide	14355709	1
Caelo	Triamcinolone acetonide	14355706	1
Caelo	Triamcinolone acetonide	15233904	12
Caelo	Triamcinolone acetonide	14233904	1
Fargon	Triamcinolone acetonide	15C19-B06-308572	2
Caelo	Triamcinolone acetonide	14355701	1
EuRho	Triamcinolone acetonide	150800-08-02	1
EuRho	Triamcinolone acetonide	1508008-02	2
Euro OTC	Triamcinolone acetonide	1508008-02	12
Caelo	Triamcinolone acetonide	14G23B072976618	1
Fargon	Triamcinolone acetonide	15C19-B06-308573	1
Euro OTC	Triamcinolone acetonide	15233904	1
Newchem/Noweda	Triamcinolone acetonide	15C19-B06-308573	1
Oberlinden Apotheke	Triamcinolone acetonide	B0544/114010	1
Fagron	Triamcinolone acetonide	14F30-B021-296287	1
Gehe	Triamcinolone acetonide	15B02-B03-303827	1
Fagron	Triamcinolone acetonide	15B02-B03-303828	1
Fagron	Triamcinolone acetonide	15C19-B06-308573	7
AHD	Triamcinolone acetonide	14355711	1
WE: 08.12.2015	Triamcinolone acetonide	14K14-B05-302887	1
sanacorp	Triamcinolone acetonide	15233902	1
Noweda	Triamcinolone acetonide	15233902	1
NEWCHEM S.P.A.	Triamcinolone acetonide	NV0994M	1
Newchem S.P.A	Triamcinolone acetonide	1508008-02	1
Fagron	Triamcinolone acetonide	15C19-B06-309194	2
Caelo	Triamcinolone acetonide	15233906	13
Euro OTC	Triamcinolone acetonide	1601021-01	19
Fagron	Triamcinolone acetonide	15G31-B07-314047	2
Fagron	Triamcinolone acetonide	15G31-B07-313596	6
Fagron	Triamcinolone acetonide	1531-07-313596	1
Caelo	Triamcinolone acetonide	15233903	17
Fagron	Triamcinolone acetonide	15G31-B07-313597	5
Caelo	Triamcinolone acetonide	15233908	2
EuRho/Noweda	Triamcinolone acetonide	1601021-01	1
Ichtyol/Gehe	Triamcinolone acetonide	15430102	3
apoident	Triamcinolone acetonide	1508008-01	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Triamcinolone acetonide	150800802	2
Fagron	Triamcinolone acetonide	15G31-B07-314045	5
Noweda	Triamcinolone acetonide	15233903	1
Caelo	Triamcinolone acetonide	1504007-01	1
Sittig	Triamcinolone acetonide	1508008-02	1
Caelo	Triamcinolone acetonide	14355712	5
Fagron	Triamcinolone acetonide	15G31-B07	1
Caelo	Triamcinolone acetonide	1508008-02	1
Fagron	Triamcinolone acetonide	15g31-b07-314046	1
Caelo	Triamcinolone acetonide	15L21-B03-316123	1
Fagron	Triamcinolone acetonide	15G31B07	2
Phoenix	Triamcinolone acetonide	14355709	1
Caelo	Triamcinolone acetonide	15430103	5
Fagron	Triamcinolone acetonide	15G31-B07-314046	2
Fagron	Triamcinolone acetonide	15B02-B03-303827	2
Newchem S.p.A./Caesar &...	Triamcinolone acetonide	1543015	1
Caelo	Triamcinolone acetonide	15430105	6
Euro OTC	Triamcinolone acetonide	80616-5	1
Fagron	Triamcinolone acetonide	15B02-B03-303828	1
Caelo	Triamcinolone acetonide	5430105	1
Caelo	Triamcinolone acetonide	160102101	1
Caelo	Triamcinolone acetonide	15430102	1
Fagron	Triamcinolone acetonide	15L21-B03-316123	6
Fagron	Triamcinolone acetonide	16B04-B07-318957	6
Euro OTC	Triamcinolone acetonide	1605010-01	25
Fagron	Triamcinolone acetonide	15C19-B06	1
Caelo	Triamcinolone acetonide	160501001	1
Fagron	Triamcinolone acetonide	12/-N09	1
Caelo	Triamcinolone acetonide	15430106	5
Fagron	Triamcinolone acetonide	16B04-B07	4
Sanacorp	Triamcinolone acetonide	15430108	1
Euro OTC	Triamcinolone acetonide	15233906	2
Fagron	Triamcinolone acetonide	16B04-B07-318664	3
Caelo	Triamcinolone acetonide	15430108	7
phönix	Triamcinolone acetonide	15430107	1
Fagron	Triamcinolone acetonide	16B04-B07-319471	4
Caelo	Triamcinolone acetonide	1605010-01	1
Caelo	Triamcinolone acetonide	15L21-B03-318663	1
Anzag	Triamcinolone acetonide	1605010-01	1
Fagron	Triamcinolone acetonide	16D14-B11-321318	3
Euro OTC	Triamcinolone acetonide	160501001	1
Audor Pharma	Triamcinolone acetonide	APU0544/31524T	1
phönix	Triamcinolone acetonide	15233906	1
Euro OTC	Triamcinolone acetonide	161006T	1
Euro OTC	Triamcinolone acetonide	15L21-B03-316123	1
Caelo	Triamcinolone acetonide	15G31-B07-314045	1
phönix	Triamcinolone acetonide	1605010-01	1
Caelo	Triamcinolone acetonide	15430107	10
Caelo	Triamcinolone acetonide	16092504	15
Euro OTC	Triamcinolone acetonide	1608005-01	31
Gehe/EuRo	Triamcinolone acetonide	1605010-01	1
Noweda	Triamcinolone acetonide	1605010-01	1
Gehe	Triamcinolone acetonide	15430102	1
Fagron	Triamcinolone acetonide	16D14-B11-322158	6
Caelo	Triamcinolone acetonide	16094501	7
Phönix	Triamcinolone acetonide	1608005-01	1
Caelo	Triamcinolone acetonide	16094507	3
Fagron	Triamcinolone acetonide	1608005-01	1
Euro OTC	Triamcinolone acetonide	16D14-B11-322136	1
Fagron	Triamcinolone acetonide	16D14-B11-322136	4

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Supplier	Substance	Batch	Spectra
Caelo	Triamcinolone acetonide	16094506	5
Fagron	Triamcinolone acetonide	16D14-B11-322135	4
Calo/Sanacorp	Triamcinolone acetonide	16092504	1
Caelo	Triamcinolone acetonide	1608005-01	2
Caelo	Triamcinolone acetonide	16094511	14
Newchem/Fiebig	Triamcinolone acetonide	1605010-01	1
Fagron	Triamcinolone acetonide	15L21-B03-318663	2
Gehe	Triamcinolone acetonide	160800501	1
Caelo	Triamcinolone acetonide	16094505	1
Caelo	Triamcinolone acetonide	16094504	2
Euro OTC	Triamcinolone acetonide	1608005	1
AHD 22.12.16 EK 29,74	Triamcinolone acetonide	16D14B11322136	1
Fagron	Triamcinolone acetonide	16D14-B11-325479	5
Caelo	Triamcinolone acetonide	16094514	10
Allianz Healthcare	Triamcinolone acetonide	16080005-01	1
Caelo	Triamcinolone acetonide	16094512	2
Fagron	Triamcinolone acetonide	16D14-B11	1
GEHE	Triamcinolone acetonide	1605010-01	1
Gehe/Fragon	Triamcinolone acetonide	16D14-B11-325479	1
Euro OTC	Triamcinolone acetonide	1612014-01	37
Fagron	Triamcinolone acetonide	16014-B12-3231318	1
Fagron	Triamcinolone acetonide	16B04	1
Fagron	Triamcinolone acetonide	16D14-B11-325481	1
Caelo	Triamcinolone acetonide	1612014-01	6
Caelo	Triamcinolone acetonide	170324T1612014-01	1
Phoenix WE 16.03.17 EK...	Triamcinolone acetonide	1612014-01	1
Fagron	Triamcinolone acetonide	16D14-B11-325482	2
Gehe	Triamcinolone acetonide	16094501	1
apo ident	Triamcinolone acetonide	1612014-01	1
EuRho	Triamcinolone acetonide	NW2518M	1
Audor Pharma	Triamcinolone acetonide	15240T	1
Caesar & Loretz GmbH	Triamcinolone acetonide	17057906	1
Fagron	Triamcinolone acetonide	16B04-Bo7-318664	1
Caelo	Triamcinolone acetonide	1504007-2	1
Fagron	Triamcinolone acetonide	16D14-B11-325480	3
Euro/Noweda	Triamcinolone acetonide	161201401	1
Noweda	Triamcinolone acetonide	16094514	1
EuRho / Phoenix	Triamcinolone acetonide	1612014-01	1
Caelo	Triamcinolone acetonide	17057902	8
Fagron	Triamcinolone acetonide	16K07-B06-329446	1
Euro OTC	Triamcinolone acetonide	1612014-014	1
Caelo	Triamcinolone acetonide	17057901	6
Caelo	Triamcinolone acetonide	1530102	1
Fagron	Triamcinolone acetonide	16B04-B07318664	1
Caelo	Triamcinolone acetonide	17057906	9
Caelo	Triamcinolone acetonide	17057903	2
Fagron	Triamcinolone acetonide	NW2261M	1
Caelo	Triamcinolone acetonide	17057908	14
Caelo	Triamcinolone acetonide	16K07-B06-329447	1
Fagron	Triamcinolone acetonide	16K07-B06-329445	2
Fagron	Triamcinolone acetonide	16D14B11328167	1
Caelo	Triamcinolone acetonide	16D14-B11	1
Audor Pharma	Triamcinolone acetonide	APU0544/3162705	1
Audor Pharma	Triamcinolone acetonide	APU0544/315240T	2
Ebert/Euo	Triamcinolone acetonide	1612014-01	1
Kehr	Triamcinolone acetonide	1057902	1
Fagron	Triamcinolone acetonide	16D04-B11-325479	1
Caelo	Triamcinolone acetonide	17057905	7
Euro OTC	Triamcinolone acetonide	NW2518M	1
Newchem Spa (site)	Triamcinolone acetonide	16K07-B06-332102	1

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Supplier	Substance	Batch	Spectra
Noweda	Triamcinolone acetonide	1608005-01	1
Fagron	Triamcinolone acetonide	16D14-B11-328167	8
Euro OTC	Triamcinolone acetonide	1703037-01	21
Caelo	Triamcinolone acetonide	170547902	1
Euro OTC	Triamcinolone acetonide		2
Euro OTC	Triamcinolone acetonide	1703037	2
Noweda	Triamcinolone acetonide	17057908	1
Caelo	Triamcinolone acetonide	16094513	1
Noweda	Triamcinolone acetonide	17057905	2
Finteler Apotheke	Triamcinolone acetonide	17057910	1
Fagron	Triamcinolone acetonide	16K07-B06-332101	6
Fagron	Triamcinolone acetonide	16D14-B11322158	1
Fagron	Triamcinolone acetonide	16D14B11325479	1
Caelo	Triamcinolone acetonide	16K07-B06-333438	3
GEHE	Triamcinolone acetonide	16K07-B06-332103	1
Caelo	Triamcinolone acetonide	17057907	2
Caelo	Triamcinolone acetonide	17120603	10
Fagron	Triamcinolone acetonide	16-B07-318664	1
Noweda	Triamcinolone acetonide	1703037-01	2
Caesar & Loretz GmbH	Triamcinolone acetonide	17057907	1
Euro OTC	Triamcinolone acetonide	1706013-01	25
Fagron	Triamcinolone acetonide	16K07-B06-333438	2
GEHE	Triamcinolone acetonide	1706013-01	1
Caelo	Triamcinolone acetonide	17120605	3
Fagron	Triamcinolone acetonide	17C09-B01-337464	2
Caelo	Triamcinolone acetonide	16079502	1
Caelo	Triamcinolone acetonide	17120606	7
Phoenix	Triamcinolone acetonide	1703037-01	1
Caelo	Triamcinolone acetonide	17057909	2
Euro OTC	Triamcinolone acetonide	171212T/1703037-01	1
Fagron	Triamcinolone acetonide	NX0241M	1
EuRho/ Sanacorp	Triamcinolone acetonide	1703037-01	1
GEHE	Triamcinolone acetonide	1710002-01	1
Fagron	Triamcinolone acetonide	17C09-B01337464	1
Fagron	Triamcinolone acetonide	16K07-B06-332102	3
Fagron	Triamcinolone acetonide	17C09-B01-334196	2
almirall/gehe	Triamcinolone acetonide	17120607	2
Caelo	Triamcinolone acetonide	17120611	10
Caelo	Triamcinolone acetonide	17120619	5
Fagron	Triamcinolone acetonide	17C09-B01	2
Caelo	Triamcinolone acetonide	1706013-01	2
Fagron	Triamcinolone acetonide	17C09-B01-334197	1
Euro OTC	Triamcinolone acetonide	171613-01	1
Audor Pharma	Triamcinolone acetonide	APU0544/316270T	2
Caelo	Triamcinolone acetonide	17120608	4
Caelo	Triamcinolone acetonide	17128606	1
Noweda	Triamcinolone acetonide	17120606	2
Euro OTC	Triamcinolone acetonide	1710002-01	23
Caelo	Triamcinolone acetonide	17120618	5
Caelo	Triamcinolone acetonide	17120607	2
Caelo	Triamcinolone acetonide	17120610	6
Fagron	Triamcinolone acetonide	17C09-B01-340173	2
Noweda	Triamcinolone acetonide	17120611	1
Caelo	Triamcinolone acetonide	17120604	3
Fagron	Triamcinolone acetonide	17H03-B12-343458	3
Euro / Noweda	Triamcinolone acetonide	1612014-01	1
Fagron	Triamcinolone acetonide	17C09-B01-336881	1
Fagron	Triamcinolone acetonide	17C09-B01-340174	2
Fagron	Triamcinolone acetonide	17H03-B12-343457	2
Bombastus	Triamcinolone acetonide	17120611	1

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Supplier	Substance	Batch	Spectra
EuRho/Noweda	Triamcinolone acetonide	1710002-01	1
Caelo	Triamcinolone acetonide	17120620	4
Euro OTC	Triamcinolone acetonide	17100002-01	1
Phönix W.E: 16.04.2018 ...	Triamcinolone acetonide	1710002-01	1
Gehe/EuRo	Triamcinolone acetonide	1801020-01	1
Fagron	Triamcinolone acetonide	17H03-B12-343672	4
Newchem S. p. A. / Noweda	Triamcinolone acetonide	17120608	1
Sanacorp	Triamcinolone acetonide	17120603	1
Caelo	Triamcinolone acetonide	17358302	12
EuroOCT/Gehe	Triamcinolone acetonide	1710002-01	2
Euro OTC	Triamcinolone acetonide	170303701	1
Sanacorp	Triamcinolone acetonide	17120610	1
Caelo	Triamcinolone acetonide	17C09-B01-340174	1
Anzag	Triamcinolone acetonide	17120605	1
Caelo	Triamcinolone acetonide	17358303	4
Fagron	Triamcinolone acetonide	17H03-B12-343459	1
Sanacorp	Triamcinolone acetonide	17358305	1
Bombastus	Triamcinolone acetonide	17120610	1
Fagron	Triamcinolone acetonide	NX1540M	1
Fagron	Triamcinolone acetonide	18C15-B05	2
Caelo	Triamcinolone acetonide	17358305	8
Euro OTC	Triamcinolone acetonide	1801020-01	9
Euro OTC	Triamcinolone acetonide	171002-01	1
Sanacorp	Triamcinolone acetonide	17H03-B12-345553	1
Fagron	Triamcinolone acetonide	17H03-B12-345552	2
Caelo	Triamcinolone acetonide	17358304	3
Fagron	Triamcinolone acetonide	18C15-B05-347275	1
Audor Pharma	Triamcinolone acetonide	APU0544/317171T	1
Fagron	Triamcinolone acetonide	17H03-B12-345553	1
Fagron	Triamcinolone acetonide	17H03-B12	1
Euro OTC	Triamcinolone acetonide	1805001-01	5
Caelo	Triamcinolone acetonide	1801020-01	3
phoenix-06.11.18	Triamcinolone acetonide	1801020-01	1
Fagron	Triamcinolone acetonide	18C15B05347275	1
Caelo	Triamcinolone acetonide	17358302-T20181115Ma	1
Jenne	Triamcinolone acetonide	18C15-B05-347275	1
Caelo	Triamcinolone acetonide	18100206	1
Sanacorp	Triamcinolone acetonide	NY0485M	2
Euro OTC	Triamcinolone acetonide	1805001-02	2
Fagron	Triamcinolone acetonide	18C15-B05-349087	1
Caelo	Triamcinolone acetonide	18100204	2
Caelo	Triamcinolone acetonide	18100203	2
Fagron	Triamcinolone acetonide	18c15-b05-349087	1
Fagron	Triamcinolone acetonide	18C15-B05-350263	1
Fagron	Triamcinolone acetonide	1810015-01	1
Euro OTC	Triamcinolone acetonide	1810015-01	1

- 77 297 spectra from 565 *Apo-Ident* customers from a total of 25 766 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Triamcinolone acetonide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this

purpose, all relevant spectra of the various substances were compared with *Triamcinolone acetonide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	497	0	73 999
Type B	0	963	0	125 929
Type C	0	1622	10	77 297

The substance/substance group *Triamcinolone acetonide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.7928 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 99.3769 %)
Type C	100.0000 % (> 99.8817 %)	99.3873 % (> 99.2034 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20765	20765	0.00	7.84
21962	21587	2.40	6.51
21587	21587	0.00	8.55
21061	21061	0.00	6.17
21072	21061	2.01	6.15
22572	22572	0.00	9.03
22313	22313	0.00	7.20
22752	22752	0.00	6.49
20910	21061	1.89	6.84
21883	21883	0.00	6.66

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Triamcinolone, micronized**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20564-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Triamcinolone, micronized; Triamcinolonum micronisatum

Special notes

When selecting the *Triamcinolone, micronized* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Triamcinolone, micronized*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Triamcinolone, m...	12A03-N09	20730	40	20120117
Fagron	Triamcinolone, m...	12K07-N13	20936	80	AR-15-FG-003373-01
Caelo	Triamcinolone, m...	15106905	22273	30	20150527
Fagron	Triamcinolone, m...	14B13-B30-316101	22840	40	20140311
Fagron	Triamcinolone, m...	17G03-B04-343670	24097	40	1807456

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Triamcinolone, m...	17G03-B04-343670	24107	40	20171101
Fagron	Triamcinolone, m...	18A19-B05-351174	24182	40	1811263
Fagron	Triamcinolone, m...	18A19-B05-351174	24182SI	32	1811263

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 342 spectra of 8 reference samples from the substance/substance group *Triamcinolone, micronized*. These samples are listed above in the [calibration samples](#) section.
- 74154 spectra from a total of 1617 batches from further 372 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 [†].

- 255 spectra of 7 reference samples from the substance/substance group *Triamcinolone, micronized*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Triamcinolone, micronized	15106905	22273 [†]	15
Caelo	Triamcinolone, micronized	15106905	22605	40
Caelo	Triamcinolone, micronized	15106911	23508	40
Fagron	Triamcinolone, micronized	18E09-B04-353921	24446	40
Fagron	Triamcinolone, micronized	17G03-B04-343670	24097SI	40
Fagron	Triamcinolone, micronized	17G03-B04-343670	24107SI	40
Fagron	Triamcinolone, micronized	18E09-B04-353921	24446SI	40

- 126637 spectra from a total of 2785 batches from further 781 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](#).

[†]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.

- 24 spectra from 19 *Apo-Ident* customers from 20 batches from the substance/substance group *Triamcinolone, micronized*.

Supplier	Substance	Batch	Spectra
Fagron	Triamcinolone, micronized	11D28-N04	1
Fagron	Triamcinolone, micronized	11G26-N04	1
Fagron	Triamcinolone, micronized	12A03-N09	1
Fagron	Triamcinolone, micronized	13C26-N04	1
Fagron	Triamcinolone, micronized	12Do2-N14	1
Fagron	Triamcinolone, micronized	12F01-N19	2
Fagron	Triamcinolone, micronized	13D30-N15	2
Caelo	Triamcinolone, micronized	14B13-B30-293474	1
Caelo	Triamcinolone, micronized	13J07-N08	2
Caelo	Triamcinolone, micronized	12295210	1
Noweda 24.08.2015	Triamcinolone, micronized	14B13-B30-293474	1
Fagron	Triamcinolone, micronized	12D02-N14	1
Fagron	Triamcinolone, micronized	14B13-B30-316102	1
Caelo	Triamcinolone, micronized	15106960	1
Fagron	Triamcinolone, micronized	14B13-B30-312868	1
Fagron	Triamcinolone, micronized	15B13-B30-312868	1
Caelo	Triamcinolone, micronized	15106902	1
Sanacorp	Triamcinolone, micronized	15106916	1
Fagron	Triamcinolone, micronized	16A13-B06	1
Fagron	Triamcinolone, micronized	14B13-B30	1
Fagron	Triamcinolone, micronized	14B13-B30-293473	1

- 78 905 spectra from 565 *Apo-Ident* customers from a total of 26 118 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Triamcinolone, micronized* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Triamcinolone, micronized* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	342	0	74 154
Type B	0	175	80	126 637
Type C	0	21	3	78 905

The substance/substance group *Triamcinolone, micronized* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.2456 %)
Type B	100.0000 % (> 99.9901 %)	68.6275 % (> 67.4510 %)
Type C	100.0000 % (> 99.8817 %)	87.5000 % (> 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
20936	20936	0.00	62.28
20730	20936	24.78	50.26
22273	20936	7.96	63.06
24097	24097	0.00	22.05
24107	24097	0.73	22.71
22840	20936	10.18	58.65
24182	24182	0.00	13.55

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Triclosan**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20005-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Triclosan; Triclosanum

Special notes

When selecting the *Triclosan* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Triclosan*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Triclosan	13391808	21509	40	20131211
Caelo	Triclosan	14121209	21591	30	20140718
Euro OTC	Triclosan	1406032-01	21615	40	20140710
Euro OTC	Triclosan	1507041	21856	40	20150804*
Euro OTC	Triclosan	1510045	22227	40	20150511*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Triclosan	1602003	22373	30	20160204*
Euro OTC	Triclosan	1701032	22987	40	20170207*
Fagron	Triclosan	17K02-B06-343548	23915	40	20180105

Validation samples

A total of 280 317 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 *Triclosan*. These samples are listed above in the [calibration samples](#) section.
- 74 196 spectra from a total of 1615 batches from further 372 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 [†].

- 490 spectra of 15 reference samples from the substance/substance group *Triclosan*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Triclosan	13391808	21509 [†]	20
Caelo	Triclosan	14121209	21591 [†]	15
Euro OTC	Triclosan	1406032-01	21615 [†]	20
Euro OTC	Triclosan	1507041	21856 [†]	20
Euro OTC	Triclosan	1510045	22227 [†]	20
Euro OTC	Triclosan	1602003	22373 [†]	15
Caelo	Triclosan	160846	22453	60
Euro OTC	Triclosan	1607002	22674	40
Caelo	Triclosan	162808	22775	40
Caelo	Triclosan	171498	23315	40
Euro OTC	Triclosan	1705011	23425	40
Euro OTC	Triclosan	1708025	23699	40
Euro OTC	Triclosan	1801049	23964	40
Caelo	Triclosan	180814	24048	40
Caelo	Triclosan	182537	24387	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*).

- 126 402 spectra from a total of 2774 batches from further 781 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.

- 2223 spectra from 455 *Apo-Ident* customers from 417 batches from the substance/substance group *Triclosan*.

Supplier	Substance	Batch	Spectra
Fagron	Triclosan	10J18-N01	2
Caelo	Triclosan	11076716	1
Caelo	Triclosan	11238003	2
Fargon	Triclosan	4394403	1
Fagron	Triclosan	11H09-N02	6
EuRho	Triclosan	1107030-01	2
Caelo	Triclosan	11238009	2
Fagron	Triclosan	4394083	1
Caelo	Triclosan	12c21-n05	1
Caelo	Triclosan	12003201	3
DAB 2008	Triclosan	12003201	2
Fagron	Triclosan	11238004	1
Fagron	Triclosan	C12H7C1302	1
Euro OTC	Triclosan	4486611	2
Fagron	Triclosan	11L19-N11	6
Caelo	Triclosan	12003205	7
Gehe	Triclosan	11J28-N02	1
EuRho	Triclosan	1202018-01	1
Fagron	Triclosan	11J28-N02	4
Fagron	Triclosan	12C21-N05	22
Euro OTC	Triclosan	1107030-01	3
Euro OTC	Triclosan	1202018-01	1
Fagron	Triclosan	12G09-N09	5
Fagron	Triclosan	1209213402	1
Fargon	Triclosan	12C21-N05	1
Phoenix	Triclosan	12003202	1
Fagron	Triclosan	12c21-n05	3
Anzag	Triclosan	12G09-N09	2
Caelo	Triclosan	11076717	2
Caelo	Triclosan	12003210	5
Anzag	Triclosan	5846205	1
Fagron	Triclosan	12G17-N04	29
Fagron	Triclosan	434083	1
Caelo	Triclosan	12145901	5
Euro OTC	Triclosan	1202018-02	2
Caelo	Triclosan	12145902	5
Fagron	Triclosan	12G17-n04	1
Caelo	Triclosan	12003202	1
Caelo	Triclosan	12G17-N04	2
Anzag 4.12.12 ek:8,89	Triclosan	12G17-N04	1

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Hence, these spectra are not independent and are not of *Type B*.

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Supplier	Substance	Batch	Spectra
Caelo	Triclosan	5012E-03402	1
Caelo	Triclosan	12145906	6
Caelo	Triclosan	12145910	11
Fagron	Triclosan	2901313402	1
Caelo	Triclosan	12145908	7
Fagron	Triclosan		4
Phönix	Triclosan	12145908	1
fargon	Triclosan	12G17-N04	1
Fagron	Triclosan	11A05-N13	1
Fagron	Triclosan	12G17N04	1
Euro OTC	Triclosan	1206034-02	3
Anzag	Triclosan	12G17-N04	3
Fagron	Triclosan	12L06-N01	31
Caelo	Triclosan	20021304	1
Caelo	Triclosan	12145909	10
Fagron	Triclosan	5846205	2
Fagron	Triclosan	12g17-n04	2
Krieger	Triclosan	12g17-N04	1
Caelo	Triclosan	11238011	1
Caelo	Triclosan	12145907	9
Caelo	Triclosan	1125204	1
Gehe	Triclosan	12145910	1
Euro OTC	Triclosan	120203-02	1
Fagron	Triclosan	11D20-N10	1
Caelo	Triclosan	12L06-N01	7
Caelo	Triclosan	12L06-N01/0005900346	1
Bombastus	Triclosan	12L06-N01	2
Fagron	Triclosan	13a11n03	1
Fagron	Triclosan	13A11-N03	10
Caelo	Triclosan	12145917	1
Alliance Healthcare	Triclosan	12G09-N09	1
Euro OTC	Triclosan	1211025-01	11
Gehe	Triclosan	12106-n01	1
Euro OTC	Triclosan	1206034-01	1
A.H.D.	Triclosan	12L06-N01	1
Caelo	Triclosan	12359104	6
BASF Grenzach/Noweda	Triclosan	5900346	1
Alliance Healthcare	Triclosan	12L06-N01	1
Caelo	Triclosan	12359110	5
Caelo	Triclosan	13D02-N02	7
Gehe	Triclosan	13A11-N03	1
Fagron	Triclosan	13A11N03	1
Fagron	Triclosan	13D02-N02	64
Caelo	Triclosan	12106-n01	1
Caesar/Lorenz	Triclosan	12145910	1
Caesar/Lorenz	Triclosan	12359104	1
Fagron	Triclosan	12106-n01	1
BASF Chem trade GmbH/Ph...	Triclosan	5846205	1
Fagron	Triclosan	2513Q-03402	1
agron/ Noweda	Triclosan	13A11-N03	1
Caelo	Triclosan	12359105	7
Caelo	Triclosan	12359111	7
Noweda	Triclosan	12359107	1
Sanacorp	Triclosan	12359105	2
Caelo	Triclosan	12359108	13
BASF Grenzach GmbH/Phönix	Triclosan	13A11-N03	1
Gehe	Triclosan	12359105	1
Bombastus	Triclosan	12359111	1
Fagron	Triclosan	12G09-no9	1
Caelo	Triclosan	11238004	1

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Supplier	Substance	Batch	Spectra
Gehe	Triclosan	12359104	1
Euro OTC	Triclosan	1303011-01	5
Phönix	Triclosan	12L06-N01	1
Caelo	Triclosan	13A11-N03	2
Fargon	Triclosan	13D02-N02	2
Noweda	Triclosan	12G17-N04	2
Caelo	Triclosan	12359106	11
Fagron	Triclosan	13D02N02	1
Caelo	Triclosan	12359107	1
Fischar/Gehe	Triclosan	13D02-N02	1
AHC 02.09.13 EK9,04	Triclosan	13D02-N02	1
Fagron	Triclosan	13Do2-N02	1
Phönix	Triclosan	12359111	1
Caelo	Triclosan	12359112	8
Fagron	Triclosan	13092012C	1
BASF Grenzach GmbH/Phönix	Triclosan	13A11-No3	1
Fagron	Triclosan	13H08-N10	30
Caelo	Triclosan	AKD12	1
Europ Ots Pharma	Triclosan	13D02-N02	1
Caelo	Triclosan	12359109	3
Sanacorp	Triclosan	12359106	1
Fagron	Triclosan	90000383	1
Phönix	Triclosan	12359109	1
Eigenproduktion	Triclosan	13A11-N03	1
Phönix	Triclosan	13A11-N03	1
Caelo	Triclosan	13D02-No2	1
Alliance Healthcare	Triclosan	13D02-N02	1
Euro OTC	Triclosan	1307050-01	5
Noweda	Triclosan	13247903	1
BASF Grenzach GmbH/Phönix	Triclosan	13D02-N02	1
Sanacorp	Triclosan		1
Caesar/Lorenz	Triclosan	13247904	1
anzag 20.11.2013	Triclosan	12359114	1
Fagron	Triclosan	13D02-N02	1
Fagron	Triclosan	13d02-N02	1
Caelo	Triclosan	13247903	1
Euro OTC	Triclosan	CHB1303011-01	1
Fagron	Triclosan	13H08N10	2
Caelo	Triclosan	12359114	1
Caelo	Triclosan	13247905	10
Fagron	Triclosan	13H09-N01	57
Gehe	Triclosan	13D02-N02	1
Gehe	Triclosan	12359112	1
sana corp	Triclosan	12359106	1
Caelo	Triclosan	13247904	11
Caelo	Triclosan	13247908	2
Sanacorp	Triclosan	13D02-N02	1
Fagron	Triclosan	6012014E	1
Caelo	Triclosan	13247805	1
Sanacorp	Triclosan	13247904	2
Caelo	Triclosan	13H09-N01	7
Caelo	Triclosan	13H08-N10	2
Gehe	Triclosan	12359114	1
Caelo	Triclosan	16021306	1
Fagron	Triclosan	13D02-N-02	1
Fagron	Triclosan	13H08-N-10	1
Caelo	Triclosan	15121202	1
Fagro/Gehe	Triclosan	13H08-N10	1
Fagron	Triclosan	9000383	2
EuRho/Phönix	Triclosan	1307050-01	2

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Supplier	Substance	Batch	Spectra
Caeolo/Noweda	Triclosan	13247905	1
Fagron	Triclosan	14022014C	1
Caeolo	Triclosan	13391801	2
Fagron	Triclosan	13h08-n10	1
Euro OTC	Triclosan	1401038-01	9
Fagron	Triclosan	10006226	2
Fagron	Triclosan	1214I03402	1
Gehe	Triclosan	13391804	2
Euro OTC	Triclosan	13H08-N10	1
Caeolo	Triclosan	3041408	1
Caeolo	Triclosan	13391802	4
Gutenberg-Apotheke	Triclosan	13H09-N01	2
Caeolo	Triclosan	14052103	13
Fagron	Triclosan	13H09-N011296/2856	1
Caeolo	Triclosan	13391804	9
Sanacorp	Triclosan	13391807	2
Fagron	Triclosan	13L18-B35-289988	1
Caeolo	Triclosan	13391807	3
GEHE 22.04.2014	Triclosan	13391804	1
Euro OTC	Triclosan	1245	1
Fagron	Triclosan	13L18-B35-289984	4
BASF Grenzach GmbH/Phönix	Triclosan	10006226	1
Caeolo	Triclosan	14052102	11
Fagron	Triclosan	13L18-B35-289986	5
Fagron	Triclosan	13L18-B35	12
Gehe	Triclosan	13391811	1
Fagron	Triclosan	13L18B35289987	1
Caeolo	Triclosan	13391808	9
Fagron	Triclosan	13L18-B35-289	1
Fagron	Triclosan	13H08-N100450/1231	1
EuRho / 30	Triclosan	1401038-01	1
Fagron	Triclosan	13L18-B35-289983	10
Phönix Gotha	Triclosan	13391807	1
Euro OTC	Triclosan	130301101	1
BASF Grenzach GmbH/Phönix	Triclosan	13H09-N01	1
Fagron	Triclosan	160614	1
Phonix	Triclosan	13L18-B35	1
Fagron	Triclosan	10666066	2
Fagron	Triclosan	13H09-No1	1
Fagron	Triclosan	13L18-B35-289985	12
Caeolo	Triclosan	13L18-B35-289986	2
Caeolo	Triclosan	14052101	5
Fagron	Triclosan	13L18-B35-289987	6
Caeolo	Triclosan	13L18-B35-289984	1
GEHE 17.06.2014	Triclosan	14052102	1
Euro OTC	Triclosan	140103801	1
Fagron	Triclosan	2914E-03402	1
Raben-Apotheke Mildenau	Triclosan	13L18-B35-289984	2
Caeolo	Triclosan	13L18B35289993	1
Caeolo	Triclosan	8081401	1
Fagron	Triclosan	700228-0005	1
Fagron	Triclosan	18082014B	1
Alliance Healthcare/Fis...	Triclosan	13H09-N01	1
Phönix	Triclosan	13H09-N01	1
Fagron	Triclosan	13L18-B35-289993	3
Euro OTC	Triclosan	1406032-01	9
Caeolo	Triclosan	13L18-B35-289995	1
Fragron	Triclosan	13D02-N02	1
Fagron	Triclosan	13L18-B35-289995	6
Caeolo	Triclosan	14052105	1

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Supplier	Substance	Batch	Spectra
Caelo	Triclosan	14121207	9
Fagron	Triclosan	13H09N01	2
Fagron	Triclosan	13L18B35289984	1
Caelo	Triclosan	14121203	8
Caelo	Triclosan	14121209	6
Caelo	Triclosan	13L18-B35-289992	2
Fagron	Triclosan	13L18-B35-289985	1
Caelo	Triclosan	1412109	1
Gutenberg-Apotheke	Triclosan	13L18-B35	1
Sanacorp	Triclosan	26/AKD1	1
Fagron	Triclosan	13L18-B35-289994	6
noweda	Triclosan	13L18-B35-289985	1
Fagron	Triclosan	13L-18-B35-289985	1
Phönix	Triclosan	13L18-B35-289985	1
Phönix	Triclosan	13L18-B35-289995	2
Fagron	Triclosan	13L18-B35289995	1
Caelo	Triclosan	14F23B02293859	1
Phönix	Triclosan	13L8-B35	1
Fagron	Triclosan	13L18-B35-289992	2
Fagron	Triclosan	106666066	1
Fagron	Triclosan	10112014C	1
sanacorp	Triclosan	13L18-B35-289987	1
Caelo	Triclosan	14211207	1
Gehe	Triclosan	14052105	1
Phoenix 19.11.14	Triclosan	14121207	1
Alliance Health 26.11.2...	Triclosan	13L18-B35-289995	1
Sana 06.11.14 EK 3,38	Triclosan	14121209	1
Caelo	Triclosan	14121204	8
Sonnenberg-Apotheke	Triclosan	13L18-B35-289995	1
Beiersdorf	Triclosan	14F23-B02-295764	1
ebe a	Triclosan	14121207	1
Euro OTC	Triclosan	1408024-01	6
Sanacorp	Triclosan	14052103	1
Fagron	Triclosan	14F23-B02-295759	9
Nowed 18.12.2014	Triclosan	14121210	2
Apomix/Noweda	Triclosan	1406032-01	2
Caelo	Triclosan	23121409	1
Fagron	Triclosan	14F23-B02-295764	2
Caelo	Triclosan	14121220	1
Fagron	Triclosan	14F23-B02-295762	3
Caelo	Triclosan	14121210	8
Caelo	Triclosan	14121215	13
EuRho	Triclosan	1408024-01	1
Caelo	Triclosan	13L18-B35-289987	1
Fagron	Triclosan	14F23-B02	5
Anzag	Triclosan	13L18-B35-289995	1
Fagron	Triclosan	14F23-B02-293852	2
Bombastus	Triclosan	13L18-35-289984	1
Caelo	Triclosan	13L18B35289986	1
Gehe	Triclosan	1408024-01	2
Phönix Gotha	Triclosan	1408024-01	2
Alliance Healthcare	Triclosan	13L-18-835	1
Caelo	Triclosan	14F23-B02	1
Fagron	Triclosan	14F23-B02-295765	5
Fagron	Triclosan	13L18-35-289995	1
Fagron	Triclosan	14F23-B02295756	1
Gehe	Triclosan	14121210	1
AHD 17.01.15	Triclosan	13L18-B35-289992	1
Euro OTC	Triclosan	14121204	1
Fagron	Triclosan	14F-B02-293859	1

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Supplier	Substance	Batch	Spectra
Fagron	Triclosan	14F23-B02-295761	11
Caesar & Loretz/AHD	Triclosan	14121209	1
Caesar&Loretz GmbH/Anzag	Triclosan	14121215	2
Euro OTC	Triclosan	1501032-01	10
Caelo	Triclosan	14121211	8
Fagron	Triclosan	200315B	1
Fagron	Triclosan	14F23-B02-295756	2
EuRho/Phoenix	Triclosan	1401038-01	1
Fargon	Triclosan	14F23-B02-295948	1
Euro OTC	Triclosan	140603201	1
Caelo	Triclosan	14121214	10
Fagron	Triclosan	14F23-B02-295760	9
Caelo	Triclosan	14F23-B02-295765	1
Fagron	Triclosan	14F23-B02-295757	4
Fagron	Triclosan	14F23-B02-295763	3
Caelo	Triclosan	14211211	1
Caelo	Triclosan	11777748	3
Sanacorp	Triclosan	14121211	1
Gehe	Triclosan	14121211	1
Fagron	Triclosan	14F23-B02-295948	4
Fagron	Triclosan	14F23B02295763	1
Fagron	Triclosan	11777748	4
Caelo	Triclosan	14F23-B02-295760	1
Kremer/Phönix	Triclosan	15/157/T	1
Allianc.Healthc../Apomix	Triclosan	14F23-B02-295760	1
Caelo	Triclosan	14205903	11
Caelo	Triclosan	14205902	9
Noweda	Triclosan	14F23-B02-295765	1
Sanacorp	Triclosan	28/AKD4	1
Fagron	Triclosan	190615A	1
Caelo	Triclosan	14205901	5
Caelo	Triclosan	14205904	6
Caelo	Triclosan	150103201	1
Euro OTC	Triclosan	1505009-01	10
Euro OTC	Triclosan	700228	1
Euro OTC	Triclosan	150500901	1
Phoenix	Triclosan	14205903	1
Fagron	Triclosan	14F23-B02-295758	10
Caelo	Triclosan	14205905	5
Sanacorp	Triclosan	14121215	1
Sanacorp	Triclosan	1505009-01	1
Fagron	Triclosan	14F23-B02295757	1
Gehe	Triclosan	14205904	1
Caelo	Triclosan	1505009	1
Euro OTC	Triclosan	14F23-B02-295948	1
Fagron	Triclosan	14F23B02300219	1
Caelo	Triclosan	15203603	13
Fagron	Triclosan	15G07-B03-310037	13
Fagron	Triclosan	15G07-B03-310040	5
Caelo	Triclosan	15G07-B03-310037	2
Fagron	Triclosan	14F23-B02-300219	7
Noweda	Triclosan	15203603	2
Fagron	Triclosan	15G07-B03-310041	1
Caelo	Triclosan	15203608	11
Fagron	Triclosan	15G07-B03	3
Euro OTC	Triclosan	1507041-01	6
Caesar&Loretz GmbH/Anzag	Triclosan	15203603	2
Caelo	Triclosan	1520603	1
Fagron	Triclosan	15G07B03310037	1
Fagron	Triclosan	14f23-b02-295757	1

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Supplier	Substance	Batch	Spectra
Caelo	Triclosan	1507041-01	2
Caesar&loretz,Phönix	Triclosan	15203606	1
Fagron	Triclosan	15G07-B03-310038	6
Fagron	Triclosan	15G01-B03-310038	1
Caelo	Triclosan	15203606	8
Caelo	Triclosan	15203604	10
Fagron	Triclosan	TCS0214037	2
Fragron	Triclosan	15G07-B03-310040	1
Fagron	Triclosan	15G07-B03-310036	3
Caelo	Triclosan	15G07-B03-30039	1
Caelo	Triclosan	1501032-02	1
Euro OTC	Triclosan	1501032-02	4
Fagron	Triclosan	15G07-B03-310039	2
Fagron	Triclosan	14F23-B02-295947	4
Fagron	Triclosan	14f23-b02-295758	1
Caelo	Triclosan	15203607	12
caesar&loretz,Phönix	Triclosan	15203607	1
Euro OTC	Triclosan	15G07-B03-310040	1
Henry Lamotte/ Noweda	Triclosan	15203606	1
Gehe	Triclosan	1505009-01	1
Fagron	Triclosan	14F23-Bo2-295947	1
Gehe-Fragron	Triclosan	14F23B02300219	2
Gehe-Fragron	Triclosan	15G07B03310036	2
Caelo	Triclosan	15301501	1
Rondell Apotheke	Triclosan	11965460	1
Caelo	Triclosan	15301502	12
Fagron	Triclosan	15C10-B06-311161	10
Fagron	Triclosan	15C10-B06-310032	4
Fagron	Triclosan	14F23-B02-2959947	1
Euro OTC	Triclosan	1510045-01	10
Euro OTC	Triclosan	15203607	3
Euroct/Gehe	Triclosan	1510045-01	2
Fagron	Triclosan	17G07-B03-310038	1
Caesar und Loretz	Triclosan	15301502	1
Faron	Triclosan	14F23-B02-300219	2
Caelo	Triclosan	15G07-B03-310035	1
Fagron	Triclosan	15G07B03310040	1
Fagron	Triclosan	15203604	1
Caelo	Triclosan	15G07-B03-310038	1
Caelo	Triclosan	5203607	1
Fagron	Triclosan	15C10B06311161	2
Fagron	Triclosan	15C10-B06-312983	7
Caelo	Triclosan	15301505	9
Fagron	Triclosan	15c10-B06-311161	1
EuRho	Triclosan	151004501	1
Caelo	Triclosan	15301503	8
Caelo	Triclosan	15C10-B06-311161	1
Fagron	Triclosan	15C10-B06-312982	12
Noweda	Triclosan	15203604	1
Fagron	Triclosan	15C10-B06	5
Fagron	Triclosan	15C10-B06-3161	1
Caeo/Noweda	Triclosan	15301505	1
Fagron	Triclosan	15G07-B03-310035	8
Caelo	Triclosan	15C10-B06-312982	3
Euro OCT/Noweda	Triclosan	1501032-02	1
Fagron	Triclosan	15C-B06-312982	1
Fagron	Triclosan	15c10-b06-312980	1
Fagron	Triclosan	15C10-B06312980	1
Caelo	Triclosan	15301506	14
Caelo	Triclosan	15G07-B03-310035/201	1

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Supplier	Substance	Batch	Spectra
Euro UTC	Triclosan	1510045-01	1
Caelo	Triclosan	15301510	2
Kumar Organic/Noweda	Triclosan	15C10-B06	1
Fagro/Sanacorp	Triclosan	TCS0214037	1
Fagron	Triclosan	15G07	1
Euro OTC	Triclosan	1602003-01	21
Fagron	Triclosan	15C10-B06-312981	16
WE:02.04.2016 Sanacorp ...	Triclosan	15C10-B06-312982	3
Fagron	Triclosan	15C10B06312982	1
Caelo	Triclosan		1
Fagron	Triclosan	15C10-B06-310031	5
Fagron	Triclosan	15C10B06312983	1
Caelo	Triclosan	150704101	1
Caelo	Triclosan	15301512	5
Fagron	Triclosan	14F23B02295758	1
Caelo	Triclosan	15301504	8
Phoenix	Triclosan	15C10-B06	1
Caelo	Triclosan	15C10-B06-310031	3
Gehe/Fragon	Triclosan	15C10B06312981	2
Cealo/AHD	Triclosan	14F23-B02-295947	1
triclosan	Triclosan	15C10-B06-310032	1
Caelo	Triclosan	1503603	1
Caelo	Triclosan	1530105	1
Fagron	Triclosan	15C10-B06-312980	5
Caelo	Triclosan	15301511	7
Caelo	Triclosan	16084601	6
Euro OTC	Triclosan	151004501	1
Caesar&Loretz GmbH/Sana...	Triclosan	15301505	1
Euro/Gehe	Triclosan	1602003-01	1
Fagron	Triclosan	151010-B06-312984	1
Caelo	Triclosan	160084601	1
Fagron	Triclosan	15301510	1
Noweda	Triclosan	1408024-01	1
Fagron	Triclosan	15G047-B03-0001	1
Caelo	Triclosan	15301513	1
Caelo	Triclosan	16084607	10
Caelo	Triclosan	15301514	1
Caelo	Triclosan	15G07-B03-310040	1
Caelo	Triclosan	16084602	7
Caelo	Triclosan	16084603	7
Caelo	Triclosan	16084610	8
Caelo	Triclosan	160846	1
Sanacorp WE:05.09.16 ...	Triclosan	1602003-01	2
Caelo	Triclosan	16084609	2
Euro OTC	Triclosan	1607002-01	21
Phönix	Triclosan		1
Caesar & Loretz/AHC	Triclosan	16084603	2
L30/Alliance	Triclosan	1607002-01	1
Sanacorp	Triclosan	151004501	1
Caelo	Triclosan	16084606	4
Caelo	Triclosan	16084608	14
Euro OTC	Triclosan	160200301	1
Euro OTC	Triclosan	160531T	1
Euro OTC	Triclosan	160702-01	1
Caesar u Loretz	Triclosan	15301503	1
Caelo	Triclosan	16084614	13
Phoenix	Triclosan	16084614	1
Caesar&Loretz GmbH	Triclosan	16084609	1
Caelo	Triclosan	15C10-B06-310031	1
Phönix	Triclosan	1516A-03402	1

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Supplier	Substance	Batch	Spectra
Caelo	Triclosan	1602003-01	2
Caelo	Triclosan	16084611	14
Fagron	Triclosan	16084614	1
Euro OTC	Triclosan	12276023	1
Caelo	Triclosan	16084618	12
Caelo	Triclosan	16084617	1
Fagron	Triclosan	16084603	1
Gehe	Triclosan	16084614	1
Euro OTC	Triclosan	1609005-01	16
Fagron	Triclosan	15C10B06310031	2
Caesar&Loretz,AHC,12.12...	Triclosan	16084618	1
ALH	Triclosan	1607002-01	2
Euro OTC	Triclosan	15C10-B06-312981	1
Caelo	Triclosan	162808	1
Caelo	Triclosan	16280801	20
Gehe	Triclosan	16280801	2
Caelo	Triclosan	160846018	1
Caelo	Triclosan	12680801	1
Caelo	Triclosan	16084620	1
Euro OTC	Triclosan	12276024	1
Caelo	Triclosan	1607002-01	2
Euro OTC	Triclosan	170113T1609005-01	1
Euro OTC	Triclosan	16084614	1
Caelo	Triclosan	16280808	13
Caelo	Triclosan	16280810	1
Alliance Healthcare	Triclosan	16084608	1
Caelo	Triclosan	16280802	16
Phönix	Triclosan	16280801	1
Caelo	Triclosan	16280811	10
Caelo	Triclosan	517E-03402	1
EuRhoNoweda	Triclosan	1602003-01	1
Anzag	Triclosan	1607002-01	2
Caesar & Loretz GmbH	Triclosan	16280811	1
Caelo	Triclosan	16280805	1
Euro OTC	Triclosan	1609005-02	15
Phönix	Triclosan	16280811	2
Caelo	Triclosan	16280809	5
Caelo	Triclosan	16280819	5
Caelo	Triclosan	16280820	4
Caelo	Triclosan	16280816	12
Euro/Noweda	Triclosan	1607002-01	1
Gehe	Triclosan	16280811	1
Euro OTC	Triclosan	1701032-02	5
Caelo	Triclosan	1609005-02	1
Caelo	Triclosan	16280803	3
Euro OTC	Triclosan	169005-02	1
Caelo	Triclosan	1701032-01	1
Caelo	Triclosan	16280824	2
Gehe	Triclosan	16280808	1
Caelo	Triclosan	1628082	1
Euro OTC	Triclosan	1701032-01	11
Euro OTC	Triclosan	170132-01	1
Phoenix	Triclosan	1701032-01	1
Euro/Phönix	Triclosan	170103201	1
Caelo	Triclosan	17081705	6
Caelo	Triclosan	16280821	1
Caelo	Triclosan	17081704	1
Caelo	Triclosan	17081706	2
Caelo	Triclosan	16280818	4
Caelo	Triclosan	17081707	18

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Supplier	Substance	Batch	Spectra
Euro OTC	Triclosan	170526T/1701032-02	1
Caelo	Triclosan	170817075274	1
Caelo	Triclosan	17081710	13
Euro OTC	Triclosan	1701032	1
Caelo	Triclosan	2317I-03402	1
Fagron	Triclosan	17081702	1
Caelo	Triclosan	16280817	5
Gehe	Triclosan	1701032-01	1
Caelo	Triclosan	17081711	9
Caesar&Lorenz	Triclosan	17081707	1
Caleo/Phönix	Triclosan	17081711	1
GEHE	Triclosan	1701032-01	1
Caelo	Triclosan	12276827	1
Caelo	Triclosan	17081709	9
phoenix	Triclosan	17081707	2
Apotheke an der Bornhei...	Triclosan	16280817	3
Euro/Phönix	Triclosan	160900502	1
Caelo	Triclosan	162820817	1
Phoenix	Triclosan	1701032-02	1
EurRho/Gehe	Triclosan		1
Phönix Berlin / Lamotte	Triclosan	17081711	1
Caelo	Triclosan	17081703	4
Caelo	Triclosan	170817	1
GEHE	Triclosan	17081710	1
Euroo/direkt	Triclosan	1705011-01	1
Caelo	Triclosan	17081713	4
Caelo	Triclosan	17081714	4
Caelo	Triclosan	17081712	9
Noweda	Triclosan	16280818	1
Caelo	Triclosan	17081702	1
phönix	Triclosan	17081712	1
Euro OTC	Triclosan	1705011-01	16
Caelo	Triclosan	17081716	6
Caelo	Triclosan	17149805	5
Noweda	Triclosan	17081703	1
Anzag	Triclosan	1701032-02	1
Caelo	Triclosan	17081721	11
GEHE	Triclosan	1701032-02	1
Caelo	Triclosan	170501101	1
Noweda	Triclosan	17081711	1
Caelo	Triclosan	17081717	2
Caelo	Triclosan	17081725	11
Caelo	Triclosan	1705011-01	1
Sanacorp	Triclosan	17081725	1
Gehe	Triclosan	1705011-01	1
Euro OTC	Triclosan	171121T/1705011-01	1
Caelo	Triclosan	17081724	11
Caelo	Triclosan	17081722	13
Euro OTC	Triclosan	170501101	1
Caelo	Triclosan	6121711	1
Euro OTC	Triclosan	170103201	1
Euro OTC	Triclosan	17081722	1
Caelo	Triclosan	17149806	4
Cealo	Triclosan	71215/1Gie	1
Caelo	Triclosan	17149801	3
Euro OTC	Triclosan	1708025-01	13
Caelo	Triclosan	17081726	5
EuRho	Triclosan	1705011-01	1
Noweda	Triclosan	17149801	1
Caelo	Triclosan	17081716-T20180112Ma	1

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Supplier	Substance	Batch	Spectra
AHD	Triclosan	17081723	1
Caelo	Triclosan	17081723	2
Fagron	Triclosan	1708025-01	1
Phönix	Triclosan	17081725	1
Caelo	Triclosan	17081720	10
Sanacorp	Triclosan	17149806	1
Euro OTC	Triclosan	170802501	1
Caelo	Triclosan	17149809	15
Fagron	Triclosan	17K02-B06	1
Euro OTC	Triclosan	170825-01	1
Noweda	Triclosan	1705011-01	1
Bombastus	Triclosan	17081726	1
Caelo	Triclosan	170817265507	1
Caelo	Triclosan	17149807	6
Caelo	Triclosan	17149817	5
Caelo	Triclosan	17149819	9
Caelo	Triclosan	170802-01	1
Euro OTC	Triclosan	17149806	1
Euro OTC	Triclosan	1550229	1
AHL	Triclosan	1801049-01	2
Caelo	Triclosan	17149808	16
Euro OTC	Triclosan	1801049-01	3
Caelo	Triclosan	1714819	1
Caesar & Loretz/ Noweda	Triclosan	17149812	1
Caelo	Triclosan	17149813	7
Sanacorp	Triclosan	17149812	1
Caelo	Triclosan	17149812	3
Caelo	Triclosan	17149824	3
Caelo	Triclosan	171498085598	1
Sanacorp	Triclosan	17149808	1
Caelo	Triclosan	17149820	9
Sanacorp WE: 30.04.18 E...	Triclosan	1708025-01	1
BASF	Triclosan	1708025-01	1
Fiebig	Triclosan	17149819	1
Caelo	Triclosan	17149825	9
Allianz	Triclosan	1801049-01	1
Caelo	Triclosan	1714930	1
Fagron	Triclosan	17K02-B06-343548	1
Euro OTC	Triclosan	180149-01	1
Caeolo	Triclosan	17149809	1
Caelo	Triclosan	17149812-20180619Ma4	1
Caelo	Triclosan	17149827	5
Caelo	Triclosan	18081402	2
Caelo	Triclosan	16071801	1
Cealo/Gehe	Triclosan	17149807	1
Caelo	Triclosan	17149814	2
Caelo	Triclosan	18081401	2
Caelo	Triclosan	18081403	5
Fagron	Triclosan	17149814	3
Noweda/EuRo	Triclosan	1801049-01	1
Fiebig	Triclosan	17149814	1
Fagron	Triclosan	17K02-B06-343547	3
Caelo	Triclosan	17149821	10
Caelo	Triclosan	17149815	5
Caesar & Loretz GmbH	Triclosan	17149821	1
Caelo	Triclosan	17149822	3
Caelo	Triclosan	10206240	1
Sanacorp	Triclosan	17149814	1
Delta Apotheke	Triclosan	17149822	1
Caelo	Triclosan	18081407	4

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Supplier	Substance	Batch	Spectra
Caelo	Triclosan	18081406	5
Klosterring	Triclosan	18081405	1
Caelo	Triclosan	17149813-T20181115Ma	1
Caelo	Triclosan	18081405	9
Caelo	Triclosan	1719814	1
Caelo	Triclosan	18081408	6
Caelo	Triclosan	18081410	2
Caelo	Triclosan	18081415	4
Sanacorp	Triclosan	18081415	1
Caeolo/Phönix	Triclosan	18081416	1
Caelo	Triclosan	18081413	3
Caelo	Triclosan	18081416	1
Euro OTC	Triclosan	1901006-01	2

- 76 706 spectra from 565 *Apo-Ident* customers from a total of 25 725 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Triclosan* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Triclosan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 196
Type B	0	490	0	126 402
Type C	0	2177	46	76 706

The substance/substance group *Triclosan* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.7755 %)
Type C	100.0000 % (> 99.8817 %)	97.9307 % (> 97.7958 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21509	22373	2.40	75.20
21591	22373	3.19	74.08
21615	22373	4.76	73.61
21856	21856	0.00	74.49
22227	22227	0.00	73.55
22373	22373	0.00	74.98
22987	22987	0.00	73.24
23915	22987	6.95	74.88

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Trometamol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20004-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Trometamol; Trometamolum

Special notes

When selecting the *Trometamol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Trometamol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Trometamol	13E22-N05	20856	40	AR-17-FG-016395-01
Caelo	Trometamol	14050002	21358	40	20140220
Caelo	Trometamol	161688	22629	40	20160615*
Caelo	Trometamol	16168810	23498	40	20160615

Validation samples

A total of 280 317 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 *Trometamol*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 *Trometamol*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Trometamol	17A16-B04-334121	23516	40
Fagron	Trometamol	17A16-B04-334121	23517	40
Caelo	Trometamol	173208	23787	40
Euro OTC	Trometamol	1803016	24063	40

- 126 732 spectra from a total of 2786 batches from further 781 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.

- 479 spectra from 249 *Apo-Ident* customers from 116 batches from the substance/substance group *Trometamol*.

*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
Caelo	Trometamol	11160706	1
Caesar & Loretz GmbH, 4...	Trometamol	11160714	1
Gehe	Trometamol	11160708	1
Caelo	Trometamol	11376005	5
Noweda	Trometamol	11376005	1
Caelo	Trometamol	11160707	1
Caelo	Trometamol	11376006	8
Caelo	Trometamol	26111201	1
Caelo	Trometamol	11160714	2
Caelo	Trometamol	1001312519	1
Caelo	Trometamol	213E-02519	1
Fagron	Trometamol	12I27-No3	1
Sanacorp	Trometamol	12113506	1
Caelo	Trometamol	12113506	8
Caelo	Trometamol	12113502	3
Caelo	Trometamol	12113505	1
Fagron	Trometamol	294101	1
Caelo	Trometamol		3
Anzag	Trometamol	12113512	1
Caelo	Trometamol	12113512	10
Gehe	Trometamol	11025103	1
Fagron	Trometamol	12K14-N05	2
ANZAG	Trometamol	12113512	1
Fagron	Trometamol	12k14no5	1
Fagron	Trometamol	13C08-N07	3
Phönix	Trometamol	12113512	1
Euro OTC	Trometamol	1203005-02	3
Caelo	Trometamol	12113515	4
Caelo	Trometamol	13095901	9
Caelo	Trometamol	12113511	1
Caelo	Trometamol	12113507	3
Caelo	Trometamol	12113510	1
Caelo	Trometamol	11160711	1
Fagron	Trometamol	12I27-N03	1
Caelo	Trometamol	13095902	10
Fagron	Trometamol	13E22-N05	5
Klenk	Trometamol	13095902	2
Caelo	Trometamol	21082013A	1
Caelo	Trometamol	13095910	5
Caesar & Loretz GmbH, 4...	Trometamol	13095902	1
Gehe	Trometamol	13E22-N05	1
Caelo	Trometamol	13095905	1
Caelo	Trometamol	13095911	12
Caelo	Trometamol	27111304	1
AHD	Trometamol	13095910	1
Fagron	Trometamol	13I19-B02	1
Caelo	Trometamol	13095912	14
Caelo	Trometamol	13095913	3
Fagron	Trometamol	13/19-B02-286158	3
Phönix	Trometamol	13095912	2
Fagron	Trometamol	13I19-B02-286158	1
Caelo	Trometamol	314Q2519	1
Fagron	Trometamol	8386E050	1
Fagron	Trometamol	13/19-B02	1
Caelo	Trometamol	8031301	1
Caelo	Trometamol	13095915	3
Fagron	Trometamol	13I19-B02-286158	1
Merck	Trometamol	8386F017	1
Phönix Gotha	Trometamol	1319-B02-286158	1
Caelo	Trometamol	13339103	7

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Supplier	Substance	Batch	Spectra
Sanacorp	Trometamol	13095912	1
Caelo	Trometamol	5012M-02519	1
Caelo	Trometamol	13339107	7
Anzag	Trometamol	13095911	1
Caelo	Trometamol	1339103	1
Caelo	Trometamol	13051401	1
Caelo	Trometamol	13339108	11
Caelo	Trometamol	14050002	7
Caelo	Trometamol	13C-08-N07	1
Fagron	Trometamol	12E25-B40	1
Caelo	Trometamol	3713E-02519	1
Phönix Gotha	Trometamol	13/19-B02-286158	1
Caelo	Trometamol	14050003	2
Caelo	Trometamol	14050004	3
Caelo	Trometamol	914I-02519	1
Caelo	Trometamol	14050006	1
Sanacorp	Trometamol	3686G018	1
Caesar & Loretz GmbH	Trometamol	14050003	1
Fagron	Trometamol	610I-02519	1
Caelo	Trometamol	14332402	21
Fagron	Trometamol	13/19-B02-293595	2
Phönix	Trometamol	14332402	1
Caelo	Trometamol	23062015B	1
Caelo	Trometamol	14332403	1
Caelo	Trometamol	15094401	13
Caelo	Trometamol	14332404	1
Caelo	Trometamol	18081503	1
Caelo	Trometamol	15070304	9
Caelo	Trometamol	15094404	1
Caelo	Trometamol	15070308	23
Caelo	Trometamol	215I-02519	1
Fagron	Trometamol	13119-B02	1
Caelo	Trometamol	15070307	4
Caelo	Trometamol	15070311	17
Caelo	Trometamol	1180116	1
Caelo	Trometamol	150703	1
Fagron	Trometamol	14F19-B03-304293	3
Caelo	Trometamol	15070309	1
Caelo	Trometamol	15377602	15
Sanocorp WE:21.05.16 EK...	Trometamol	15070311	2
Sanacorp	Trometamol	15377602	1
Caelo	Trometamol	15277602	1
Fagron	Trometamol	14F19-B03	1
Caelo	Trometamol	15377607	20
Caelo	Trometamol	15377605	1
Caelo	Trometamol	15377604	1
Caelo	Trometamol	161013T/15377607	1
Caelo	Trometamol	4616M-02519	1
Caelo	Trometamol	5315I-02519	1
Caelo	Trometamol	16168807	1
Caelo	Trometamol	15377611	14
Gehe	Trometamol	15377611	1
Caelo	Trometamol	16168812	1
Caelo	Trometamol	16168810	17
Caelo	Trometamol	16168801	1
GEHE	Trometamol	16168810	1
Caelo	Trometamol	16168820	14
Caelo	Trometamol	16168819	9
Fagron	Trometamol	17A16-B04-334121	2
Sanacorp	Trometamol	8386H037	1

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Supplier	Substance	Batch	Spectra
Caelo	Trometamol	16168816	2
Caelo	Trometamol	16168825	1
Phoenix/Cealo	Trometamol	16168825	1
Fagron	Trometamol	17A16-B04	1
Caelo	Trometamol	17197804	6
Fargon/Kehr	Trometamol	17A16-B04-337589	1
Caelo	Trometamol	17020304	5
Caelo	Trometamol	17320801	16
Fagron	Trometamol	16D14-B09-328729	1
Sanacorp	Trometamol	16168820	1
Caelo	Trometamol	171978	1
Caelo	Trometamol	17197809	2
Caelo	Trometamol	18041815	1
Caelo	Trometamol	17320801/1160518	1
AHD	Trometamol	17320801	1
Sanacorp	Trometamol	17320804	1
Caelo	Trometamol	17320804	7
Jenne	Trometamol	17320811	1
Caelo	Trometamol	17320811	8
Bombastus	Trometamol	17320811	1
Fagron	Trometamol	18A23-B10-349673	1

- 78 450 spectra from 565 *Apo-Ident* customers from a total of 26 022 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Trometamol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Trometamol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	160	0	126 732
Type C	0	473	6	78 450

The substance/substance group *Trometamol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	98.7474 % (> 98.1211 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20856	20856	0.00	35.28
21358	22629	4.89	35.19
22629	22629	0.00	36.21
23498	22629	6.74	36.82

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tropicamide**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20598-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tropicamide; Tropicamidum

Special notes

When selecting the *Tropicamide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tropicamide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tropicamide	14D23-B04-293294	21685	40	AR-15-FG-001641-01
Fagron	Tropicamide	16G19-B05-324829	22885	40	20160905
Fagron	Tropicamide	17J06-B04-341322	23982	40	1807428

Validation samples

A total of 280 317 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 *Tropicamide*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Tropicamide*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Tropicamide	14D23-B04-293294	21685 [†]	20
Fagron	Tropicamide	17D25-B07-336833	23506	40
Audor Pharma	Tropicamide	APFP/TD003/09/17/TR	23983	40

- 126 792 spectra from a total of 2786 batches from further 781 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 8 *Apo-Ident* customers from 11 batches from the substance/substance group *Tropicamide*.

Supplier	Substance	Batch	Spectra
Fagron	Tropicamide	20021302	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	Tropicamide	12F18-N06	4
Fagron	Tropicamide	12104-n03	1
Fagron	Tropicamide	14D23B04293294	1
Fagron	Tropicamide	23071508	1
Gehe	Tropicamide	15F-18B-04	1
Gehe	Tropicamide	15F18-B04	1
Phoenix	Tropicamide	14L04-B02	2
ALH	Tropicamide	15F18-B04-310971	1
Fagron	Tropicamide	14104-b02-315694	1
Fagron	Tropicamide	15F18-B04-308977	1

- 78 914 spectra from 565 *Apo-Ident* customers from a total of 26 126 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tropicamide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tropicamide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	100	0	126 792
Type C	0	15	0	78 914

The substance/substance group *Tropicamide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.8817 %)	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
21685	21685	0.00	39.45
22885	23982	7.62	36.87
23982	23982	0.00	37.18

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tyrosine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21574-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tyrosine; Tyrosinum

Special notes

When selecting the *Tyrosine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tyrosine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tyrosine	13G24-N22	21574	40	1411030
Fagron	Tyrosine	16B26-B01-322911	23533	40	20160324

Validation samples

A total of 280 317 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 *Tyrosine*. These samples are listed above in the [calibration samples](#) section.
- 74 416 spectra from a total of 1621 batches from further 372 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 *Tyrosine*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Tyrosine	13G24-N22	21574 [†]	20
Euro OTC	Tyrosine	L1401037-01	21586	60
Fagron	Tyrosine	17B06-B03-338139	24008	40

- 126 772 spectra from a total of 2786 batches from further 781 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 *Tyrosine*.

Supplier	Substance	Batch	Spectra
Euro OTC	Tyrosine	L1401037	1
Euro OTC	Tyrosine	L1210050-01	1
Euro OTC	Tyrosine	L1506022-02	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*.

- 78 926 spectra from 565 *Apo-Ident* customers from a total of 26 134 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tyrosine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tyrosine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 416
Type B	0	103	17	126 772
Type C	0	2	1	78 926

The substance/substance group *Tyrosine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9901 %)	85.8333 % (> 83.3333 %)
Type C	100.0000 % (> 99.8821 %)	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
21574	21574	0.00	82.12
23533	21574	8.68	75.27

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Tyrothricin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20732-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tyrothricin; Tyrothricinum

Special notes

When selecting the *Tyrothricin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Tyrothricin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tyrothricin	12K14-N01	20732	40	1509178
Fagron	Tyrothricin	12K14-N01	21683	40	AR-15-FG-001172-01
Fagron	Tyrothricin	14A23-B05-294146	21876	40	AR-15-FG-015005-01

Validation samples

A total of 280 317 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 *Tyrothricin*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1621 batches from further 372 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 [†].

- 186 spectra of 5 reference samples from the substance/substance group *Tyrothricin*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Tyrothricin	12K14-N01	21683 [†]	20
Fagron	Tyrothricin	14A23-B05-294146	21876 [†]	20
Fagron	Tyrothricin	17E09-B03-341231	23742	40
Fagron	Tyrothricin	12K14-N01	21683SI	60
Fagron	Tyrothricin	14A23-B05-294146	21876SI	46

- 126 706 spectra from a total of 2786 batches from further 781 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 5 *Apo-Ident* customers from 6 batches from the substance/substance group *Tyrothricin*.

[†]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
Fagron	Tyrothricin	15A06-B02-303893	1
Fagron	Tyrothricin	15A06-B02-3005	1
Fagron	Tyrothricin	13A14-N04	1
Fagron	Tyrothricin	15A06-B02-323005	3
Fagron	Tyrothricin	17E09-B03	1
Fagron	Tyrothricin	17E09-B03-351982	1

- 78 921 spectra from 565 *Apo-Ident* customers from a total of 26 131 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tyrothricin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tyrothricin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	180	6	126 706
Type C	0	8	0	78 921

The substance/substance group *Tyrothricin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	96.7742 % (> 95.1613 %)
Type C	100.0000 % (> 99.8818 %)	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
20732	20732	0.00	39.32
21683	21683	0.00	36.54
21876	21876	0.00	37.14

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Ubidecarenone**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20392-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ubidecarenone; Ubidecarenonum

Special notes

When selecting the *Ubidecarenone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Ubidecarenone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ubidecarenone	1205029-01	21247	40	20121009
Caelo	Ubidecarenone	14004504	21388	40	AR-15-FG-009220-01
Euro OTC	Ubidecarenone	1605030	22696	40	20160623*
Euro OTC	Ubidecarenone	1703026	23127	40	20170406*
Caelo	Ubidecarenone	17209402	23581	40	20170823
Euro OTC	Ubidecarenone	1801019	23881	40	20180126*

Validation samples

A total of 280317 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 *Ubidecarenone*. These samples are listed above in the [calibration samples](#) section.
- 74256 spectra from a total of 1617 batches from further 372 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 [†].

- 295 spectra of 8 reference samples from the substance/substance group *Ubidecarenone*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ubidecarenone	14004504	21388 [†]	20
Fagron	Ubidecarenone	16G26-B01-331742	23161	40
Caelo	Ubidecarenone	17209402	23580	40
Caelo	Ubidecarenone	172094	23647	35
Euro OTC	Ubidecarenone	1802025	24074	40
Euro OTC	Ubidecarenone	1804020	24116	40
Caelo	Ubidecarenone	182298	24281	40
Euro OTC	Ubidecarenone	1810012	24305	40

- 126597 spectra from a total of 2781 batches from further 781 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.

- 11 spectra from 7 *Apo-Ident* customers from 11 batches from the substance/substance group *Ubidecarenone*.

Supplier	Substance	Batch	Spectra
Euro OTC	Ubidecarenone	L1403020-01	1
Fagron	Ubidecarenone	14H26-B04-298244	1
Euro OTC	Ubidecarenone	1403020-02	1
Fagron	Ubidecarenone	14E12-B06-293861	1
Euro OTC	Ubidecarenone	1014E-07029	1
Euro OTC	Ubidecarenone	1515M-07029	1
Fagron	Ubidecarenone	16G26-B01	1
Audor Pharma	Ubidecarenone	APSCFQ150614C	1
Audor Pharma	Ubidecarenone	APSZFQ150614C	1
Dr. Behr	Ubidecarenone	WE18020018	1
Caelo	Ubidecarenone	18048401	1

- 78 918 spectra from 565 *Apo-Ident* customers from a total of 26 126 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ubidecarenone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ubidecarenone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	295	0	126 597
Type C	0	8	3	78 918

The substance/substance group *Ubidecarenone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.9661 %)
Type C	100.0000 % (> 99.8818 %)	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
21247	23127	2.56	55.80
21388	21388	0.00	57.50
22696	22696	0.00	57.92
23127	23127	0.00	56.48
23581	21388	1.81	57.33
23881	23881	0.00	55.66

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Urea**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20017-2019-05-24
Executing company HiperScan GmbH
 Weieritzstrae 3
 01067 Dresden
 Germany

Relevant substance names

Urea; Carbamidum

Special notes

When selecting the *Urea* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
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Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Urea*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Urea	12F25-N05	20712	40	20120724
Euro OTC	Urea	1404024-01	21537	40	20140519
Caelo	Urea	15154103	22315	40	20150722
Fagron	Urea	14I18-B03-303581	22317	40	20141003
Caelo	Urea	161074	22466	40	20160509*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Urea	170216	23033	40	20170202*
Caelo	Urea	18023003	24294	40	20180216
Caelo	Urea	15154103	22315SI	40	20150722
Fagron	Urea	14I18-B03-303581	22317SI	40	20141003

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Urea*. These samples are listed above in the [calibration samples](#) section.
- 74136 spectra from a total of 1616 batches from further 372 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 [†].

- 680 spectra of 20 reference samples from the substance/substance group *Urea*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Urea	1404024-01	21537 [†]	20
Caelo	Urea	15154103	22315 [†]	20
Fagron	Urea	14I18-B03-303581	22317 [†]	20
Euro OTC	Urea	1601044	22376	40
Caelo	Urea	161074	22466 [†]	20
Euro OTC	Urea	1604044	22552	40
Euro OTC	Urea	1702023	23156	40
Euro OTC	Urea	1707015	23535	40
Caelo	Urea	180242	24042	40
Caelo	Urea	180230	24043	40
Euro OTC	Urea	1804007	24078	40
Euro OTC	Urea	1811012	24340	40
Caelo	Urea	15154103	22315SI [†]	20
Fagron	Urea	14I18-B03-303581	22317SI [†]	20
Euro OTC	Urea	1604044	22552SI	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	Urea	170216	23033SI	40
Euro OTC	Urea	1702023	23156SI	40
Euro OTC	Urea	1804007	24078SI	40
Caelo	Urea	18023003	24294SI	40
Euro OTC	Urea	1811012	24340SI	40

- 126 212 spectra from a total of 2775 batches from further 781 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.

- 1907 spectra from 472 *Apo-Ident* customers from 296 batches from the substance/substance group *Urea*.

Supplier	Substance	Batch	Spectra
Caelo	Urea	13064226	12
Fagron	Urea	11H01-N08	2
Caelo	Urea	11150722	3
Bombastus	Urea	11150721	1
Caelo	Urea	11150725	3
Caesar & Loretz GmbH, 4...	Urea	11150736	1
Caelo	Urea	11150736	4
Caesar&lorenz,Phoenix	Urea	11150713	1
Caelo	Urea	12111802	8
Caelo	Urea	10081208	1
Caesar & Loretz GmbH, 4...	Urea	12111804	1
Gutenberg-Apotheke	Urea		1
Caelo	Urea	12111804	4
Caesar&lorenz,Anzag	Urea	11150738	1
Caesar&Loretz GmbH D-40...	Urea	12111808	2
Caelo	Urea	2109212544	1
Caelo	Urea	11150721	1
Fagron	Urea	12C20-N05	1
Caelo	Urea	12111808	9
Caelo	Urea	11150713	1
Caelo	Urea	12111806	5
Caesar&lorenz,Phoenix	Urea	12111806	3
Caelo	Urea	12111801	4
Euro OTC	Urea	1110023-01	1
Caelo	Urea	11150702	2
Sanacorp	Urea	12111808	2
Caelo	Urea	10116	1
Caelo	Urea	21111806	1
Caelo	Urea	12111810	13
Caelo	Urea	1211804	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	Urea	4111M-02544	1
Caelo	Urea	10169726	2
Anzag	Urea	12111801	1
Caelo	Urea	12111807	5
Finze	Urea	1264	1
Caesar & Loretz GmbH, 4...	Urea	12111810	2
Fagron	Urea	11F24-N16	1
Caelo	Urea	1211808	1
Caelo	Urea	12111809	12
Caelo	Urea	20130912-4	1
Gehe	Urea	12111810	1
Caelo	Urea	12111820	12
Fagron	Urea	12F25-N05	3
Caelo	Urea	11150714	1
Caelo	Urea	12111822	15
Sanacorp	Urea	12111810	1
Caelo	Urea	1211806	1
Noweda	Urea	11150714	1
Gehe	Urea	12111808	1
Noweda	Urea	4109M-02544	1
Fagron	Urea	1211822	1
Caesar & Loretz GmbH	Urea	12111822	1
Caelo	Urea	12111823	9
Gehe	Urea	12111822	1
Caelo	Urea	10169722	1
Caesar & Loretz GmbH, 4...	Urea	12111828	2
Caelo	Urea	30031304	1
Caelo	Urea	3012A-02544	1
Caelo	Urea	12111828	19
Caelo	Urea	12L10-N08	1
Phönix	Urea	12111822	1
Caesar/Noweda	Urea	12111823	1
Sanacorp	Urea	12111820	1
Caelo	Urea	12111803	1
Anzag 17.04.13 ek:6,84EUR	Urea	12111823	1
Caelo	Urea	12111826	6
Fagron	Urea	12I04-N06	1
Fagron	Urea	12110-n08	1
Caelo	Urea	21051304	1
Caelo	Urea	1211820	1
Caelo	Urea	123456	2
Caesar & Loretz GmbH, 4...	Urea	12111822	1
Fagron	Urea	12104-N06	1
Caelo	Urea	13064203	11
Caelo	Urea	107063	1
Löns Apotheke	Urea	20349	1
Caesar/Lorenz	Urea	12111822	1
Fagron	Urea	13D03-N01	9
Caelo	Urea	12111834	2
Phönix Gotha	Urea	13064202	1
Caesar & Loretz GmbH	Urea	13064203	1
Caelo	Urea	13064206	18
Sanacorp	Urea	1110023-01	1
Caelo	Urea	1211809	1
Caelo	Urea	13064202	12
Gehe	Urea	12111826	1
Caelo	Urea	13064201	6
Anzag / Noweda	Urea	13064206	1
Fagron	Urea	12L10-N08	5
Caelo	Urea	26071304	1

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Supplier	Substance	Batch	Spectra
Fagron	Urea	13D03-N001	1
Caelo	Urea	11150738	1
Caesar/Noweda	Urea	13064208	1
Caesar & Loretz GmbH, 4...	Urea	13064206	2
Alliance Healthcare	Urea	12111823	1
Caesar & Loretz GmbH	Urea	13064206	1
Sanacorp	Urea	13064212	1
Sanacorp	Urea	13064203	1
Fagron	Urea	3613M-02544	1
Caelo	Urea	2324534	1
Caelo	Urea	13064212	23
Caelo	Urea	1364212	1
Euro OTC	Urea	1212007-01	6
Fagron	Urea	235/12I04-N06	1
Caelo	Urea	4013Q2544	1
Caesar&Loretz GmbH/Anzag	Urea	13064217	1
Caesar & Loretz GmbH, 4...	Urea	13064212	3
Caelo	Urea	13064207	17
Caelo	Urea	AKD6	1
Caelo	Urea	11150703	1
Caelo	Urea	17101310	1
Caelo	Urea	1306412	1
Caelo	Urea	13E21-N05	1
Hirsch	Urea	810811	1
Fagron	Urea	13E21-N05	2
Phönix	Urea	13064207	1
Caelo	Urea	9240908	1
Caelo	Urea	13064215	21
Caesar & Loretz GmbH	Urea	1306421	1
Noweda/KremerGmbH	Urea	13064201	1
Dr. August Wolff	Urea	13E17N02	1
Fagron	Urea	13E17-N02	1
Caelo	Urea	13064213	5
Caelo	Urea	13064224	2
Caelo	Urea	13064214	13
Caelo	Urea	13064223	30
Phönix	Urea	13064215	1
Fagron	Urea	13J17-B02-287604	5
Caelo	Urea	13064217	1
Fagron	Urea	13J17-B02-287602	2
Audor Pharma	Urea	PU145	1
Caelo	Urea	17011405	1
Caelo	Urea	314Q2544	1
Caelo	Urea	13064221	6
EuRho	Urea	1212007-01	1
Phönix Gotha	Urea	1212007-01	1
Caelo	Urea	62/AKD49	1
Fagron	Urea	13J17-B02	2
Phönix	Urea	13064223	1
Caelo	Urea	13064228	22
Euro OTC	Urea	1212007-02	3
Sanacorp	Urea	13064223	1
Sanacorp	Urea	1212007	1
test	Urea	test	1
Noweda	Urea	13064223	1
Caelo	Urea	1113A-025	1
Caelo	Urea		7
Caesar & Loretz GmbH	Urea	13064223	1
Caelo	Urea	13064232	14
Laborchemie Apolda/Jenn...	Urea	12345	1

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Supplier	Substance	Batch	Spectra
Fagron	Urea	13L20-B03-289708	5
Fagron	Urea	13L20-B03289708	1
Fagron	Urea	13J17B02-287604	1
Gehe	Urea	13064232	1
Caelo	Urea	13064227	5
Fagron	Urea	11C25-N01	1
PHOENIX 02.05.2014	Urea	13J17-B02-287602	2
Phönix Gotha	Urea	V096/2012	1
Caelo	Urea	1306422	1
Sanacorp	Urea	62/AKD50s	1
Euro OTC	Urea		1
Caelo	Urea	5061410	1
Caelo	Urea	13064231	9
Caelo	Urea	13064230	15
Gutenberg-Apotheke	Urea	13064227	1
Caelo	Urea	13064236	8
Euro OTC	Urea	1404024-01	11
Caelo	Urea	13064233	15
Fagron	Urea	14E07-B05-293469	8
Löns Apotheke	Urea	40003	1
Raben-Apotheke Mildenau	Urea	13J17-B02-287604	2
Cealo/Phönix	Urea	13064231	1
Fagron	Urea	13L20B03	1
Caelo	Urea	14E07-B05-293469	1
Caesar u Loretz	Urea	12111828	1
PHOENIX 29.08.2014	Urea		1
Fagron	Urea	14E07-B05	8
Caelo	Urea	14107102	27
Caelo	Urea	14E07-B05-289706	1
Caelo	Urea	1317B02-287602	1
Phoenix	Urea	13064231	1
Fagron	Urea	14E-07-B05-293469	1
AHD	Urea	14E07-B05-293469	1
Caelo	Urea	14107103	8
Sanacorp	Urea	63/AKD1	1
Euro OTC	Urea	72/14	1
Euro OTC	Urea	13064239	1
anzag	Urea	14E07-B05-293469	1
Caelo	Urea	13064239	2
Caelo	Urea	5100	1
Euro OTC	Urea	14107101	2
Phönix	Urea	13064236	1
Raben-Apotheke Mildenau	Urea	13J17-Bo2-287604	1
Sanacorp	Urea	14107102	1
Fagron	Urea	14E07-B05-289706	1
Fagron	Urea	14E07B05	3
Caelo	Urea	14107101	7
Caelo	Urea	14107109	19
Fagron	Urea	14E8900-0001	1
Sanacorp	Urea	1405028-01	1
Eurho	Urea	1404024-01	1
Fargon/Alliance HC	Urea	14E07-B05-293469	1
Fagron	Urea	14E07-B07-293469	1
Caelo	Urea	14107113	17
Caelo	Urea	5208	1
Caelo	Urea	14011513	1
Fagron	Urea	14E07-B05-297167	5
Phönix	Urea	14107109	1
Caesar&Loretz GmbH/Anzag	Urea	13064231	1
Caelo	Urea	14107112	16

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Supplier	Substance	Batch	Spectra
Fagron	Urea	14E07B05293469	1
Ph.Eur.7.0	Urea	14107109	1
Fagron	Urea	14E07-B05-297165	2
Caelo	Urea	14107108	10
Gehe	Urea	14107112	1
Caelo	Urea	14107117	8
Kirsch Pharma GmbH/Noweda	Urea	14E07-B05-293469	1
Bombastus	Urea	14107108	1
Fagron	Urea	2014162937	3
VDL;05.02.15;10.15EUR	Urea	14107113	1
Caelo	Urea	20031514	1
Träger	Urea	14107112	1
Alliance health	Urea	14E07-B05-297167	1
Noweda	Urea	14107101	1
Phönix Gotha	Urea	1404024-01	1
Caelo	Urea	14107119	21
Caelo	Urea	13042015B	1
Caelo	Urea	14107118	7
Euro OTC	Urea	14107108	1
Caelo	Urea	14107120	8
Fargon	Urea	14e07-b05-297165	1
Sanacorp	Urea	14107112	1
Caesar & Loretz GmbH	Urea	15087105	1
Caelo	Urea	15087105	11
Euro OTC	Urea	1503042-01	24
Caelo	Urea	63/AKD4	1
Fagron	Urea	14107117	1
Caesar&Loretz GmbH /Anzag	Urea	14107113	1
Caelo	Urea	14107122	15
Caelo	Urea	15087102	7
Caelo	Urea	15087103	16
Euro OTC	Urea	150304201	1
Caelo	Urea	13072015B	1
Fagron	Urea	14I18-B03	4
Caesar & Loretz GmbH	Urea	15087103	1
Gehe	Urea	15087103	1
ACM	Urea	KNC1795J14	1
Caelo	Urea	25082015A	1
Caelo	Urea	15087107	15
Caelo	Urea	14/18-B03-303581	2
Phönix	Urea	15087110	1
Caelo	Urea	15087110	21
Caelo	Urea	14197118	1
Caelo	Urea	1508/104	1
ACM	Urea	KNC0557J15	3
Fagron	Urea	14118-B03-0303581	1
Caelo	Urea	15087104	14
Anzag/Henry Lamotte	Urea	13-18-B03-303581	1
Fagron	Urea	14/18-B03-303581	6
Gehe	Urea	15087107	2
Caelo	Urea	4914I-02544	1
Fagron	Urea	14I18-B03-303581	3
Beyvers/AHD	Urea	15087104	1
Fagron	Urea	14/18-B03-303576	1
Fagron	Urea	14I18-B03-303576	4
Caesar&Loretz/Caesar&Lo...	Urea	15154104	1
Fagron	Urea	13/17-1302-287602	1
Caelo	Urea	15154104	72
Calo/AHD	Urea	15154104	1
Caelo	Urea	15154103	42

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Supplier	Substance	Batch	Spectra
EuRho	Urea	150304201	1
Caelo	Urea	14I18-B03	1
Caesar & Loretz GmbH	Urea	15154104	1
Euro OTC	Urea	15154103	2
Fagron	Urea	1418b03303581	1
Caelo/Noweda	Urea	14107112	1
Caesar&Loretz GmbH /Anzag	Urea	15087110	1
Fagron	Urea	1418B03303581	1
Fagron	Urea	14118-B03	1
Euro OTC	Urea	1515404	1
Fagron	Urea	15154104	2
Caelo	Urea	15154107	20
Castor/Phönix	Urea	15154104	1
Fagron	Urea	18-B03-303581	1
Euro OTC	Urea	1601044-01	21
Caelo	Urea	1515404	1
Noweda	Urea	15154110	1
Caelo	Urea	15154110	30
Caelo	Urea	160125/2	1
Caelo	Urea	15154101	1
Beiersdorf AG	Urea	14/18-B03-303576	1
Caelo	Urea	151541	2
Fagron	Urea	14/18B03303581	1
Caelo	Urea	15154109	6
Phoenix	Urea	15154113	1
Caelo	Urea	15154111	34
Caelo	Urea	15154113	19
Phönix	Urea	15154113	1
Caelo	Urea	2116A-02544	1
Caesar&Loretz GmbH	Urea	14107101	1
Fagron	Urea	13064233	1
Caelo	Urea	14I18-B03-303581	1
phönix	Urea	15154111	1
Caesar&Loretz GmbH	Urea	15154111	1
Caelo	Urea	15154112	28
Fagron	Urea	16D22-B02	3
WE:Phoenix 11.08.16 E...	Urea	15154111	1
phönix	Urea	15154103	2
Caelo	Urea	568900	1
Caelo	Urea	1514110	2
Caelo	Urea	160620UP	1
phönix	Urea	15154112	2
Fagron	Urea	16D22-B02-322532	3
Euro OTC	Urea	160104401	1
Fagron	Urea	16D22-B02-3221532	1
Beiersdorf	Urea	15154112	1
Fagron	Urea	2016142709	3
Fagron	Urea	16D22-B02-322526	2
Caelo	Urea	4116M-02544	1
Euro OTC	Urea	1604044-01	21
Fagron	Urea	16D22-B02-322426	1
Caelo	Urea	15154116	11
Caelo	Urea	1236	1
Dr.Wolff	Urea	1234567	1
Gehe	Urea	15154112	1
Caelo	Urea	1514107	1
Bombastus	Urea	1601044-01	1
Caelo	Urea	16107407	23
Caelo	Urea	16107406	18
Caelo	Urea	151541111	1

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Supplier	Substance	Batch	Spectra
Caelo	Urea	16107405	7
ACM	Urea	KNC0236J16	2
Fagron	Urea	16D22-802-326481	1
Fagron	Urea	16D22-B02-326481	6
Euro OTC	Urea	160404401	1
Caelo	Urea	1610407	1
Caelo	Urea	10038587	2
Caelo	Urea	16107412	50
Caelo	Urea	1514112	1
Caelo	Urea	16107413	7
Caelo	Urea	161074	2
Caelo	Urea	16107411	21
Anzag	Urea	16107411	1
phönix	Urea	16107412	2
Euro OTC	Urea	15154104	1
Caesar&Loretz GmbH,Phön...	Urea	16107411	1
Gehe,05.04.17, 5,30EUR	Urea	16107412	1
Caelo	Urea	1517E-02544	1
Caelo	Urea	19041703	1
Euro OTC	Urea	16107411	1
Fagron	Urea	16I13-B02	1
Caelo	Urea	17021601	3
Caelo	Urea	16107417	18
Caelo	Urea	1222	1
GEHE	Urea	16107412	1
Gehe	Urea	16107412	2
Caelo	Urea	170509UP/16107407	1
Euro OTC	Urea	16107412	1
Cordes/Noweda	Urea	17021601	1
Caelo	Urea	16107416	13
Fagron	Urea	16I13-B02-330166	1
Caelo	Urea	16107418	18
Gehe/Fragon	Urea	16D22-B02-326481	1
Euro OTC	Urea	1702023-01	15
Phönix	Urea	16107412	2
Kehr	Urea	16107418	1
Sanacorp	Urea	16107418	2
Fagron	Urea	16107418	1
Caesar & Loretz GmbH	Urea	16107411	1
Caelo	Urea	10038593	1
Caelo	Urea	161074165325	1
Noweda	Urea	15154112	1
Finteler Apotheke	Urea	16107417	1
Caesar&Loretz GmbH	Urea	16107417	1
Caelo	Urea	16107419	5
Caelo	Urea	16107420	26
phönix	Urea	16107420	1
Noweda	Urea	16107419	3
Caelo	Urea	161072422	1
GEHE	Urea	16107416	1
Cealo	Urea	16107416	1
Caelo	Urea	6101703	1
GEHE	Urea	16107422	1
Euro OTC	Urea	1707015-01	14
Caelo	Urea	16107422	10
Noweda	Urea	16107422	1
Bombastus	Urea	16107424	2
Caelo	Urea	16107424	31
Caelo	Urea	16107423	4
Caelo	Urea	1241017	1

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Supplier	Substance	Batch	Spectra
Phönix	Urea	16107424	1
Caelo	Urea	1607422	1
Euro OTC	Urea	16I13-B02-332953	1
Gehe	Urea	16107422	1
Fagron	Urea	16107422	1
Noweda	Urea	16107416	1
Caelo	Urea	1702023-01	1
Caelo	Urea	16107425	3
Fagron	Urea	16/13-B02	1
Caecolo/Gehe	Urea	16107424	1
Caelo	Urea	16I13-B02-332953	1
gehe	Urea	16107425	1
Sanacorp	Urea	16107423	1
Caelo	Urea	16107426	6
Caelo	Urea	16107429	4
Euro OTC	Urea	16107428	1
Caelo	Urea	16107428	9
Eur	Urea	1707015-01	1
EuRho/Noweda	Urea	1707015-01	1
Caelo	Urea	14107428	1
Caelo	Urea	16107427	1
Caelo	Urea	18024202	22
Caelo	Urea	18024201	11
EuRho	Urea	1707015-01	1
Caelo	Urea	180322H/18024202	1
Euro OTC	Urea	UP250171017	1
Bombastus	Urea	1707015-01	1
Euro OTC	Urea	18024201	1
Caelo	Urea	21041802	1
Caelo	Urea	18023004	34
Noweda	Urea	18024201	1
Phönix/Gehe	Urea	18024201	2
Caelo	Urea	18023001	7
Sanacorp	Urea	18024202	1
Caelo	Urea	1802401	1
Caelo	Urea	16/13-B02-332593	1
Caelo	Urea	18023003	13
Caelo	Urea	1061801	1
Fagron	Urea	17H16-B01-342080	2
Euro OTC	Urea	1804007-01	6
Kehr	Urea	18023004	1
Caelo	Urea	17107429	1
Bombastus	Urea	18023004	1
Caelo	Urea	18023007	7
Delta	Urea	18023004	1
Caelo	Urea	1804007-01	1
Caelo	Urea	1823004	1
Caelo	Urea	180223003	1
Caelo	Urea	118023004	1
Caelo	Urea	18023006	14
Sanacorp	Urea	18023007	1
Caelo	Urea	18023003-20180830Ma2	1
Caesar & Loretz	Urea	18024201	1
THC/Phönix	Urea	18023006	1
Phoenix	Urea	18023006	1
Fagron	Urea	18A24-B07-349015	1
Caelo	Urea	18023010	9
Caelo	Urea	18023011	10
Fagron	Urea	18A24-B07-346692	1
Caesar & Loretz GmbH	Urea	18023004	1

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Supplier	Substance	Batch	Spectra
Fagron	Urea	16I13-B02-328152	1
Caelo	Urea	18023012	2
Fagron	Urea	2018163455	1
Fagron	Urea	18A24-B07-352707	1
Kehr	Urea	1802007	1
Fagron	Urea	18A24-B07-351975	1
Caesar & Loretz	Urea	18023004	1
Caelo	Urea	18G04-B03-353339	1
Fagron	Urea	18G04-B03-355378	1

- 77 022 spectra from 565 *Apo-Ident* customers from a total of 25 851 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Urea* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Urea* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	74 136
Type B	0	677	3	126 212
Type C	0	1867	40	77 022

The substance/substance group *Urea* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9901 %)	99.5588 % (> 99.1176 %)
Type C	100.0000 % (> 99.8817 %)	97.9025 % (> 97.7451 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
22317	22466	4.14	64.08
22466	22466	0.00	62.41
23033	23033	0.00	63.21
24294	22466	5.82	65.81
20712	22466	2.40	63.38
21537	22466	2.01	60.86
22315	22466	6.50	64.89

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Uridine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20744-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Uridine; Uridinum

Special notes

When selecting the *Uridine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Uridine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Uridine	11G07-N04	20744	55	1402481
Fagron	Uridine	13K18-B31-288497	21895	40	20131129
Audor	Uridine	APIB160018211AU	23529	40	20161118

Validation samples

A total of 280 317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 135 spectra of 3 reference samples from the substance/substance group *Uridine*. These samples are listed above in the [calibration samples](#) section.
- 74 361 spectra from a total of 1620 batches from further 372 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 [†].

- 145 spectra of 5 reference samples from the substance/substance group *Uridine*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Uridine	11G07-N04	20744 [†]	5
Fagron	Uridine	13K18-B31-288497	21895 [†]	20
Audor Pharma	Uridine	APIB1600169AU	23507	40
Audor Pharma	Uridine	APIB1600169AU	23507SI	40
Audor Pharma	Uridine	APIB160018211AU	23529SI	40

- 126 747 spectra from a total of 2785 batches from further 781 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 24 *Apo-Ident* customers from 21 batches from the substance/substance group *Uridine*.

[†]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
Audor Pharma	Uridine	AP721060040/5U	2
Fagron	Uridine	11G07-N04	1
Fagron	Uridine	22041301	1
Fagron	Uridine	13D29-N06	3
Sanacorp	Uridine	AP721060040/5U	1
Fagron	Uridine	16101301	1
Phönix	Uridine	721010040	1
siehe WE-Prüfprotokoll	Uridine	54/11	1
Fagron	Uridine	14051405	1
Audor Pharma	Uridine	AP30514U	4
Fagron	Uridine	13D08-N26	1
Fagron	Uridine	721110090	4
Fagron	Uridine	12091402	1
Fagron	Uridine	13K18-B31	4
Fagron	Uridine	14F02-B09-305467	7
Fagron	Uridine	14F02-B09	1
Audor Pharma	Uridine	APIB1400280AU	1
Audor Pharma	Uridine	AP30514IB1500001AXU	4
Audor Pharma	Uridine	APIB1600182AU	3
Audor Pharma	Uridine		1
Audor Pharma	Uridine	APIB1600169AU	18
Euro OTC	Uridine	APIB1600169AU	2
Audor Pharma	Uridine	APIB1600169	1

- 78 865 spectra from 565 *Apo-Ident* customers from a total of 26 116 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Uridine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Uridine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	135	0	74 361
Type B	0	125	20	126 747
Type C	0	63	1	78 865

The substance/substance group *Uridine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.5556 %)
Type B	100.0000 % (> 99.9901 %)	86.2069 % (> 84.1379 %)
Type C	100.0000 % (> 99.8817 %)	98.4375 % (> 93.7500 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20744	20744	0.00	40.97
21895	20744	3.01	41.58
23529	20744	3.61	43.74

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Valine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20405-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Valine; Valinum

Special notes

When selecting the *Valine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Valine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Valine	15A14-B07-307756	21953	40	9198
Euro OTC	Valine	1604055	22571	40	20160601*
Euro OTC	Valine	1701026	23131	40	20170222*

Validation samples

A total of 280 317 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 *Valine*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 8 reference samples from the substance/substance group *Valine*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Valine	15A14-B07-307756	21953 [†]	20
Euro OTC	Valine	1609009	22799	40
Euro OTC	Valine	1705017	23426	40
Euro OTC	Valine	1710003	23770	40
Euro OTC	Valine	1712005	23867	40
Euro OTC	Valine	1803017	24091	40
Euro OTC	Valine	1805014	24119	40
Euro OTC	Valine	1809027	24304	40

- 126 592 spectra from a total of 2781 batches from further 781 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*.

- 5 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Valine*.

Supplier	Substance	Batch	Spectra
Fagron	Valine	13B13-N05	1
Fagron	Valine	121259	1
Euro OTC	Valine	L1309029-02	1
Euro OTC	Valine	1604055-01	1
Euro OTC	Valine	1710003-01	1

- 78 924 spectra from 565 *Apo-Ident* customers from a total of 26 132 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Valine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Valine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	300	0	126 592
Type C	0	5	0	78 924

The substance/substance group *Valine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.8819 %)	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
21953	21953	0.00	66.24
22571	22571	0.00	66.57
23131	23131	0.00	68.53

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Vancomycin hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 21748-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Vancomycin hydrochloride; Vancomycini hydrochloridum

Special notes

When selecting the *Vancomycin hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Vancomycin hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Vancomycin hydro...	1407047-01	21748	40	AR-15-FG-008950-01
Euro OTC	Vancomycin hydro...	1506029	21826	40	AR-15-FG-009077-01
Euro OTC	Vancomycin hydro...	1610038	22878	40	20161208*
Audor	Vancomycin hydro...	APHAP1609006EV	23532	40	AR-18-FG-000670-01
Fagron	Vancomycin hydro...	17I18-B08-340944	24010	40	20171109
Euro OTC	Vancomycin hydro...	1810013	24325	40	20181029*

Validation samples

A total of 280317 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 *Vancomycin hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74256 spectra from a total of 1617 batches from further 372 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 8 reference samples from the substance/substance group *Vancomycin hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Vancomycin hydrochloride	1407047-01	21748 [†]	20
Euro OTC	Vancomycin hydrochloride	1506029	21826 [†]	20
Euro OTC	Vancomycin hydrochloride	1604037	22891	40
Euro OTC	Vancomycin hydrochloride	1812005	24421	40
Euro OTC	Vancomycin hydrochloride	1407047-01	21748SI	60
Euro OTC	Vancomycin hydrochloride	1506029	21826SI	60
Euro OTC	Vancomycin hydrochloride	1610038	22878SI	40
Euro OTC	Vancomycin hydrochloride	1604037	22891SI	40

- 126572 spectra from a total of 2784 batches from further 781 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.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Vancomycin hydrochloride*.
- 78 929 spectra from 565 *Apo-Ident* customers from a total of 26 137 batches from a further 694 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Vancomycin hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Vancomycin hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	251	69	126 572
Type C	0	0	0	78 929

The substance/substance group *Vancomycin hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	78.4375 % (> 77.5000 %)
Type C	100.0000 % (> 99.8817 %)	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
21748	21748	0.00	22.00
21826	21826	0.00	22.60

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22878	22878	0.00	19.48
23532	23532	0.00	23.12
24010	23532	12.03	19.57
24325	24325	0.00	19.98

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Vanillin**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20204-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Vanillin; Vanillinum

Special notes

When selecting the *Vanillin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Vanillin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Vanillin	14044413	21737	40	20140227
Fagron	Vanillin	13J01-N07	21738	40	20130926
Caelo	Vanillin	15135302	21924	40	AR-17-FG-022168-03
Caelo	Vanillin	160895	22484	40	20160421*

Validation samples

A total of 280317 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 *Vanillin*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 7 reference samples from the substance/substance group *Vanillin*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Vanillin	14044413	21737 [†]	20
Fagron	Vanillin	13J01-N07	21738 [†]	20
Caelo	Vanillin	15135302	21924 [†]	20
Caelo	Vanillin	160895	22484 [†]	20
Caelo	Vanillin	171172	23308	40
Caelo	Vanillin	17117201	23561	40
Caelo	Vanillin	173088	23805	40

- 126692 spectra from a total of 2782 batches from further 781 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*.

- 74 spectra from 60 *Apo-Ident* customers from 39 batches from the substance/substance group *Vanillin*.

Supplier	Substance	Batch	Spectra
Fagron	Vanillin	11G28-N09	1
Caesar & Loretz GmbH D-...	Vanillin	10066830	1
Caelo	Vanillin	10066830	1
Caesar & Loretz GmbH, 4...	Vanillin	12079401	1
Fagron	Vanillin	232050-0004	1
Sanacorp	Vanillin	12H09-N06	1
Fagron	Vanillin	12H09-N06	2
Caelo	Vanillin	90961269	1
Caelo	Vanillin	12079407	2
Caelo	Vanillin	112901	1
Fagron	Vanillin	8L05-N07	1
Caelo	Vanillin	10066811	1
Caelo	Vanillin	12079410	1
Hedinger/Ebert	Vanillin	13A30-N10	1
Caelo	Vanillin	12079412	2
Gehe	Vanillin	12079412	1
Caesar & Loretz GmbH, 4...	Vanillin	12079412	1
Caelo	Vanillin	12079424	2
Caelo	Vanillin	12079417	1
Fagron	Vanillin	13J01-N07	6
Fagron	Vanillin	314Q2548	1
Caelo	Vanillin	12071401	1
fargron	Vanillin	13/01-N07	1
Caelo	Vanillin	12079428	1
Fagron	Vanillin	14G02-B99-296988	1
Dr.Hollborn	Vanillin	6082015	1
Caelo	Vanillin		1
Caelo	Vanillin	15135302	1
Caelo	Vanillin	15154014	3
Caelo	Vanillin	15154006	1
Gehe/Noweda	Vanillin	15154006	1
Caelo	Vanillin	15154017	1
Rhodia GmbH/Noweda	Vanillin	12D02-N03	1
Caelo	Vanillin	14044419	2
Caelo	Vanillin	15154020	5
Caelo	Vanillin	16089501	1
Caelo	Vanillin	15227317	1
Caelo	Vanillin	16089506	7
Caelo	Vanillin	16089508	2
Gehe	Vanillin	16089506	1
Anzag	Vanillin	12H09-N06	1
Anzag	Vanillin	16089508	1
Finteler Apotheke	Vanillin	17117201	1
Klosterring	Vanillin	17117207	1
Caelo	Vanillin	1089501	1
Caelo	Vanillin	17117201	1
Caelo	Vanillin	17117207	3
Jenne	Vanillin	18073501	1
Caelo	Vanillin	18073506	1

- 78 855 spectra from 565 *Apo-Ident* customers from a total of 26 100 batches from a further 693 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 *Vanillin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Vanillin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	200	0	126 692
Type C	0	70	4	78 855

The substance/substance group *Vanillin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.8817 %)	94.5946 % (> 90.5405 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21737	21924	3.06	27.25
21738	21924	3.47	27.23
21924	21924	0.00	25.60
22484	22484	0.00	28.12

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Waxes / Fats**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20747-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Waxes / Fats; Adeps solidus; Adeps solidus W35; Cera alba; Cera flava; Cetyl palmitate 15; Cetyl palmitas 15; Cocoa butter; Hard fat in pastilles; Hard fat W35; Microcrystalline wax; Natrii laurylsulfuricum; Oleum cacao; Paraffin, hard; Paraffin, microcrystalline; Paraffinum durum in rotulis; Paraffinum microcristallinum; Sodium dodecyl sulfate; Sodium dodecyl sulphate; Wax, bleached; Wax, yellow

Special notes

When selecting the *Waxes / Fats* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Waxes / Fats*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Spinnrad	Wax, bleached	1012402004	20747	40	20121101

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cetyl palmitate 15	12331916	20865	40	1402429
Caelo	Sodium dodecyl s...	13099011	20986	40	1403108
Caelo	Hard fat in past...	12158122	21067	40	20120627
Caelo	Wax, yellow	13335507	21433	40	20131011
Caelo	Cocoa butter	13292013	21482	40	20130924
Caelo	Wax, bleached	13378619	21483	20	1509364
Caelo	Paraffin, microc...	14307104	21682	40	AR-15-FG-005277-01
Caelo	Paraffin, hard	13390413	21731	40	20131213
Caelo	Paraffin, microc...	14307106	21766	40	20141014
Caelo	Cetyl palmitate 15	14351606	21875	40	20141219
Fagron	Hard fat W35	15A07-B12-302751	21880	40	1604639
Caelo	Cetyl palmitate 15	15301703	21984	40	AR-16-FG-007435-01
Caelo	Wax, bleached	14336620	22244	40	20141125
Caelo	Wax, yellow	15317602	22245	40	20151007
Caelo	Cetyl palmitate 15	15301703	22325	40	20151013
Caelo	Paraffin, microc...	154128	22330	40	20160112*
Fagron	Hard fat W35	15A07-B12-309245	22338	40	20150115
Caelo	Cocoa butter	14348906	22348	40	20150122
Caelo	Paraffin, hard	15232004	22349	40	1702507
Caelo	Sodium dodecyl s...	15344503	22352	40	20151022
Caelo	Hard fat in past...	160278	22479	40	20160407*
Caelo	Cetyl palmitate 15	160538	22486	40	20160323*
Caelo	Wax, yellow	162750	22767	40	20161007*
Caelo	Wax, bleached	15292022	22956	40	20150827
Caelo	Cocoa butter	163165	23067	40	20161116*
Caelo	Sodium dodecyl s...	16229217	23242	40	20160809
Caelo	Sodium dodecyl s...	170955	23278	40	20170503*
Bombastus	Hard fat in past...	306363	23565	34	20161213
Fagron	Hard fat W35	16K08-B10-334910	23601	40	20161229
Caelo	Cocoa butter	17055907	23707	33	20170310

Validation samples

A total of 280317 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1207 spectra of 31 reference samples from the substance/substance group *Waxes / Fats*. These samples are listed above in the [calibration samples](#) section.
- 73289 spectra from a total of 1593 batches from further 364 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.

*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 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 [†].

- 1393 spectra of 45 reference samples from the substance/substance group *Waxes / Fats*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cetyl palmitate 15	13295919	21316	20
Caelo	Wax, yellow	13335507	21433 [†]	20
Caelo	Sodium dodecyl sulfate	13411305	21465	60
Caelo	Cetyl palmitate 15	13295919	21522	40
Caelo	Paraffin, microcrystalline	14307104	21682 [†]	20
Caelo	Paraffin, hard	13390413	21731 [†]	20
Caelo	Paraffin, microcrystalline	14307106	21766 [†]	20
Caelo	Cetyl palmitate 15	14351606	21875 [†]	20
Fagron	Hard fat W35	15A07-B12-302751	21880 [†]	20
Caelo	Cetyl palmitate 15	15301703	21984 [†]	20
Caelo	Wax, bleached	14336620	22244 [†]	20
Caelo	Wax, yellow	15317602	22245 [†]	20
Caelo	Cetyl palmitate 15	15301703	22325 [†]	20
Caelo	Paraffin, microcrystalline	154128	22330 [†]	20
Fagron	Hard fat W35	15A07-B12-309245	22338 [†]	20
Caelo	Cocoa butter	14348906	22348 [†]	20
Caelo	Paraffin, hard	15232004	22349 [†]	20
Caelo	Sodium dodecyl sulfate	15344503	22352 [†]	20
Caelo	Hard fat in pastilles	160278	22479 [†]	20
Caelo	Cetyl palmitate 15	160538	22486 [†]	20
Caelo	Wax, bleached	161631	22587	40
Fagron	Hard fat W35	15J08-B04-324959	22806	40
Caelo	Paraffin, hard	16277704	23190	40
Caelo	Sodium dodecyl sulfate	16229205	23243	40
Klenk	Wax, yellow	0290A170314	23511	40
Caelo	Wax, yellow	17011602	23512	40
Caelo	Wax, bleached	16163109	23513	40
Caelo	Cetyl palmitate 15	17043503	23560	40
Bombastus	Hard fat in pastilles	306363	23565 [†]	6
Caelo	Cetyl palmitate 15	171640	23639	40
Caelo	Sodium dodecyl sulfate	172363	23664	40
Bombastus	Hard fat in pastilles	308558	23705	40
Caelo	Cocoa butter	17055907	23707 [†]	7
Caelo	Paraffin, microcrystalline	15412801	23724	40
Caelo	Cocoa butter	173149	23795	40
Caelo	Hard fat in pastilles	173076	23814	40
Caelo	Cetyl palmitate 15	172715	23817	40
Fagron	Hard fat W35	17K09-B03-343779	24114	40
Caelo	Cetyl palmitate 15	181499	24221	40
Caelo	Cocoa butter	181351	24226	40
Caelo	Hard fat in pastilles	181479	24228	40
Caelo	Sodium dodecyl sulfate	181822	24292	40
Caelo	Wax, bleached	182391	24351	40
Caelo	Cetyl palmitate 15	182737	24356	40
Caelo	Cocoa butter	182544	24363	40

[†]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*.

- 125 499 spectra from a total of 2746 batches from further 773 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.

- 1899 spectra from 348 *Apo-Ident* customers from 622 batches from the substance/substance group *Waxes / Fats*.

Supplier	Substance	Batch	Spectra
Caelo	Wax, yellow	11017315	1
Caelo	Wax, yellow	11017318	3
Caesar & Loretz GmbH, 4...	Wax, yellow	11285008	1
Caelo	Wax, yellow	11285001	2
Caelo	Wax, yellow	10364837	1
Caelo	Wax, yellow	11308305	1
Caelo	Wax, yellow	11285015	1
Caelo	Wax, yellow	11308311	2
Caelo	Wax, yellow	12124801	4
Caelo	Wax, yellow	121248024-2015	1
Caelo	Wax, yellow	12124802	2
Noweda	Wax, yellow	280A120627	2
Bombastus	Wax, yellow	270682	3
Bombastus	Wax, yellow	267702	1
Klenk	Wax, yellow	280A110110	1
Caelo	Wax, yellow	11285014	2
Klenk	Wax, yellow	280A120627	5
Klenk	Wax, yellow	290A120627	4
Caelo	Wax, yellow	17121202	1
Caelo	Wax, yellow	18121201	1
Caelo	Wax, yellow	17121201	1
Caelo	Wax, yellow	12124807	3
Sanacorp	Wax, yellow	12257009	1
Caelo	Wax, yellow	12257009	7
Caelo	Wax, yellow	12124805	3
Caelo	Wax, yellow	12124812	8
Caelo	Wax, yellow	12257002	3
Klenk	Wax, yellow	290A110803	1
Caelo	Wax, yellow	4910A-01239	1
Caesar/Noweda	Wax, yellow	12124811	3
Euro OTC	Wax, yellow	1201012-01	1
Caelo	Wax, yellow	12124810	4
Klenk	Wax, yellow	282A120627	1
Klenk	Wax, yellow	280-A120627	1
Noweda	Wax, yellow	12124810	1
Caelo	Wax, yellow	12041303	1
Caelo	Wax, yellow	15041301	1
Caelo	Wax, yellow	12124814	2
Caelo	Wax, yellow	12257012	3
Klenk	Wax, yellow	280A130115	25
Klenk	Wax, yellow	290A081210	1
Hirsch	Wax, yellow	12257012	1
Caelo	Wax, yellow	12124816	1
Caelo	Wax, yellow	13031201	4

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Supplier	Substance	Batch	Spectra
Caelo	Wax, yellow	12367901	12
Caelo	Wax, yellow	1214816	1
Fagron	Wax, yellow	13B04-N04	2
Caelo	Wax, yellow	12257004	2
Caelo	Wax, yellow	12124817	2
Finze	Wax, yellow	10145002	1
Caelo	Wax, yellow	22071301	1
Fagron	Wax, yellow	12D23-N05	2
Caelo	Wax, yellow	12367904	5
Caelo	Wax, yellow	12257022	3
Alliance	Wax, yellow	280A130115	1
Caelo	Wax, yellow	13031206	8
Caelo	Wax, yellow	12124806	2
Caelo	Wax, yellow	10364810	1
Phönix	Wax, yellow	12367901	1
Phönix	Wax, yellow	12367904	1
Gehe	Wax, yellow	12079412	1
Caelo	Wax, yellow	12367910	11
Gehe	Wax, yellow	12367910	1
Caelo	Wax, yellow	12124811	1
Caesar & Loretz GmbH, 4...	Wax, yellow	12367901	1
Caesar & Loretz GmbH, 4...	Wax, yellow	12367910	1
Sanacorp	Wax, yellow	12367910	1
Caelo	Wax, yellow	26091302	1
Phönix	Wax, yellow	13031206	1
Caelo	Wax, yellow	12367912	3
Caelo	Wax, yellow	30101308	1
Caelo	Wax, yellow	12367911	2
Bombastus	Wax, yellow	279999	1
Caelo	Wax, yellow	12367916-3429311150	1
Caelo	Wax, yellow	12330116	1
Caelo	Wax, yellow	12367916	6
Caelo	Wax, yellow	12367921	1
Caelo	Wax, yellow	12367915	9
Caelo	Wax, yellow	13031220	3
Alliance Healthcare	Wax, yellow	290A120627	1
Caelo	Wax, yellow	11017314	1
Caelo	Wax, yellow	10121302	1
Klenk	Wax, yellow	280A13011A	1
Caesar & Loretz GmbH	Wax, yellow	12367910	1
Caelo	Wax, yellow	13031231	6
Caesar/Noweda	Wax, yellow	13031220	1
Phönix	Wax, yellow	12367915	1
Caelo	Wax, yellow	17011403	1
Caelo	Wax, yellow	30011407	1
Caelo	Wax, yellow	13335505	1
Sanacorp	Wax, yellow	13335502	1
Anzag	Wax, yellow	1462	1
Caelo	Wax, yellow	13335502	7
Caelo/Gehe	Wax, yellow	13335502	1
Caelo	Wax, yellow	4031403	1
GEHE	Wax, yellow	13335502	1
Ichthyol	Wax, yellow	13031239	1
Caelo	Wax, yellow	13335503	6
Caelo	Wax, yellow	13031239	11
Caelo	Wax, yellow	13031222	3
Caelo	Wax, yellow	13335508	1
Caelo	Wax, yellow	12367020	1
Caelo	Wax, yellow	13335507	6
Caelo	Wax, yellow	17041402	1

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Supplier	Substance	Batch	Spectra
Alliance Health 14.04.2. . .	Wax, yellow	280A130115	1
Caesar & Loretz GmbH	Wax, yellow	13031221	1
Caelo	Wax, yellow	13051401	1
Caelo	Wax, yellow	13378603	1
Caelo	Wax, yellow	1335503	1
Sanacorp	Wax, yellow	13378619	1
Caelo	Wax, yellow	133335507	1
Caelo	Wax, yellow	13378630	2
Caelo	Wax, yellow	13378619	13
Klenk	Wax, yellow	13335513	1
Caelo	Wax, yellow	13335509	2
Caelo	Wax, yellow	13335513	3
Caelo	Wax, yellow	14189901	1
PHOENIX 24.07.2014	Wax, yellow	13001206	1
Caelo	Wax, yellow	12091404	1
Sanacorp	Wax, yellow		1
Caelo	Wax, yellow	13335517	4
Caelo	Wax, yellow	14189902	2
Caelo	Wax, yellow	13378602	1
Caelo	Wax, yellow	13378634	6
Caelo	Wax, yellow	6111407	1
Caelo	Wax, yellow	13335518	2
Euro OTC	Wax, yellow	1407013-01	1
Caelo	Wax, yellow	14189905	1
Caelo	Wax, yellow	13031221	1
Bombastus	Wax, yellow	285109	1
Caelo	Wax, yellow	14189907	2
Fagron	Wax, yellow	13L02-B01-294113	2
Caelo	Wax, yellow	13378636	1
Klenk	Wax, yellow	290A140903	5
Klenk	Wax, yellow	280A140306	7
Fagron	Wax, yellow	13L02-B01-291452	1
Caelo	Wax, yellow	13378640	1
Fagron	Wax, yellow	13102-B01	1
Caelo	Wax, yellow	14189909	5
Caelo	Wax, yellow	13335516	1
Caelo	Wax, yellow	14189908	1
Caelo	Wax, yellow	13378639	3
Caelo	Wax, yellow	28011501	1
Caelo	Wax, yellow	14189912	4
Fagron	Wax, yellow	13L02-B01-294114	1
Caelo	Wax, yellow	14189915	2
Caelo	Wax, yellow	14336605	2
Caelo	Wax, yellow	20031516	1
Caelo	Wax, yellow	20031517	1
Caelo	Wax, yellow	1418915	1
Caelo	Wax, yellow	14336609	2
Caelo	Wax, yellow	14189914	4
Caelo	Wax, yellow	14336607	11
Caelo	Wax, yellow	14189913	2
Caelo	Wax, yellow	14189917	3
Phoenix goettingen 08.05	Wax, yellow	15098901	1
Caelo	Wax, yellow	14336608	3
Caelo	Wax, yellow	13061503	1
Caelo	Wax, yellow	14189919	1
Caelo	Wax, yellow	14G07-B04-300495	1
Caelo	Wax, yellow	14336618	1
Caelo	Wax, yellow	5022904	1
Caelo	Wax, yellow	20071503	1
Caelo	Wax, yellow	1436607	1

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Supplier	Substance	Batch	Spectra
Caelo	Wax, yellow	15022902	5
Caelo	Wax, yellow	14336616	8
Caelo	Wax, yellow	15022904	4
Fagron	Wax, yellow	14336616	1
Klenk	Wax, yellow	280A150528	8
Klenk	Wax, yellow	282A140306	1
Caelo	Wax, yellow	14336617	1
Fagron	Wax, yellow	14G07-B04-300495	2
Caelo	Wax, yellow	15023003	4
Caelo	Wax, yellow	15022908	9
Caelo	Wax, yellow	14336620	3
Bombastus	Wax, yellow	296261	1
Caelo	Wax, yellow	15098902	1
Caelo	Wax, yellow	1436620	1
Caelo	Wax, yellow	1436616	1
Caelo	Wax, yellow	15317602	4
Caelo	Wax, yellow	15292007	1
Caelo	Wax, yellow	15292005	5
Klenk	Wax, yellow	290A150716	3
Caelo	Wax, yellow	15022907	1
Caelo	Wax, yellow	12K20B05287421	1
Caelo	Wax, yellow	15292004	10
Noweda	Wax, yellow	150230004	1
Caelo	Wax, yellow	15023006	3
Caelo	Wax, yellow	152920004	1
Caelo	Wax, yellow	15023004	8
Euroo	Wax, yellow	1407013-01	1
Noweda	Wax, yellow	15023002	1
Caelo	Wax, yellow	15292003	2
Caelo	Wax, yellow	15317601	5
Caelo	Wax, yellow	15317607	4
Caelo	Wax, yellow	15317603	3
Sanacorp WE:18.04.16 EK...	Wax, yellow	15023004	1
Euro OTC	Wax, yellow	1503013-01	1
Caelo	Wax, yellow	1595	1
Fagron	Wax, yellow	15317603	1
Caelo	Wax, yellow	15317608	8
Caelo	Wax, yellow	15317609	9
Caelo	Wax, yellow	15317610	5
Caelo	Wax, yellow	15292014	1
Caelo	Wax, yellow	15098901	1
Phönix	Wax, yellow	15317609	1
Caelo	Wax, yellow	15292009	1
Caelo	Wax, yellow	14189920	1
Caelo	Wax, yellow	16038201	14
Caelo	Wax, yellow	15317613	5
Caelo	Wax, yellow	150622CF	1
Caelo	Wax, yellow	15317611	1
Klenk	Wax, yellow	290A151214	2
Caesar & Loretz	Wax, yellow	16038201	1
Caesar & Loretz	Wax, yellow	15317613	1
Euro OTC	Wax, yellow	16038201	1
Caelo	Wax, yellow	161202CF/15317611	1
Caelo	Wax, yellow	16038203	9
cae	Wax, yellow	15317608	1
Pharmachem	Wax, yellow	16038202	1
Bombastus	Wax, yellow	caelo	1
Caelo	Wax, yellow	16038202	13
Wachs neu	Wax, yellow		2
Caelo	Wax, yellow	16038206	13

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Supplier	Substance	Batch	Spectra
Mittelwand bio 2017	Wax, yellow	5022017	1
Phönix	Wax, yellow	16038206	1
Caelo	Wax, yellow	15292022	1
Caelo	Wax, yellow	16034206	1
Caelo	Wax, yellow	16038207	7
Caelo	Wax, yellow	19041704	1
Klenk	Wax, yellow	160311	1
phönix	Wax, yellow	16038207	1
Caelo	Wax, yellow	16038205	1
Caelo	Wax, yellow	16051702	1
Caesar & Loretz/AHD	Wax, yellow	16038206	1
Gehe	Wax, yellow	16038207	1
Caelo	Wax, yellow	16038210	4
Caelo	Wax, yellow	17011604	9
Caelo	Wax, yellow	17011605	1
Euro/Sanacorp	Wax, yellow	1708506	1
Caesar&Loretz GmbH	Wax, yellow	16038210	1
Caelo	Wax, yellow	170011602	1
Sanacorp	Wax, yellow	16038203	1
Caelo	Wax, yellow	7091704	1
Fagron	Wax, yellow	17011607	1
Caelo	Wax, yellow	17011609	6
Caelo	Wax, yellow	17011602	3
Klenk	Wax, yellow	290A170314	2
Bombastus	Wax, yellow	17011604	1
Sanacorp	Wax, yellow	17011604	2
Caelo	Wax, yellow	1701607	1
Euro OTC	Wax, yellow	17011607	1
Caelo	Wax, yellow	17011607	6
Caelo	Wax, yellow	17011619	1
Caelo	Wax, yellow	16163112	1
Caelo	Wax, yellow	170011607	2
Caelo	Wax, yellow	5121707	1
Caelo	Wax, yellow	17011611	3
Caelo	Wax, yellow	1701611	1
Klenk	Wax, yellow	190A170314	1
Caelo	Wax, yellow	17207402	10
Bombastus	Wax, yellow	290A170915	1
Caelo	Wax, yellow	17207404	2
Caelo	Wax, yellow	17011610	2
Klenk	Wax, yellow	290A170915	1
Caelo	Wax, yellow	17011612	13
Sanacorp	Wax, yellow	17011609	1
Caelo	Wax, yellow	17207403	5
Caelo	Wax, yellow	19031810	1
Caelo	Wax, yellow	17207405	1
Caelo	Wax, yellow	18049001	7
calo	Wax, yellow	17011612	1
Sanacorp	Wax, yellow	17011612	1
Bombastus	Wax, yellow	17207405	1
Caelo	Wax, yellow	18049002	2
Caelo	Wax, yellow	18049003	2
Caelo	Wax, yellow	18113501	6
Sanacorp	Wax, yellow	18113502	1
Klenk	Wax, yellow	280A171019	1
Kehr	Wax, yellow	18113501	1
Sanacorp	Wax, yellow	18113501	1
Caelo	Wax, yellow	18113506	1
Caelo	Wax, yellow	18113505	1
Caelo	Wax, yellow	18048906	1

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Supplier	Substance	Batch	Spectra
Caelo	Wax, bleached	15292003	7
Caelo	Wax, bleached	14336620	2
Klenk	Wax, bleached	280A150528	3
Phoenix	Wax, bleached	15292003	1
Caelo	Wax, bleached	1529003	1
Caelo	Wax, bleached	280A150528	1
Caelo	Wax, bleached	14336621	1
Fagron	Wax, bleached	2155	1
Caelo	Wax, bleached	15292009	2
Caelo	Wax, bleached	15292005	1
Klenk	Wax, bleached	280A160311	10
Caelo	Wax, bleached	15292010	1
Klenk	Wax, bleached	290A150716	1
Caelo	Wax, bleached	15292004	3
Caelo	Wax, bleached	15292014	13
Caelo	Wax, bleached	14336616	1
Caelo	Wax, bleached	151210CA	1
Fagron	Wax, bleached	16A28-B10-322948	1
Caelo	Wax, bleached		1
Caelo	Wax, bleached	16163101	1
Pharmachem	Wax, bleached	15292014	1
Caelo	Wax, bleached	15292022	4
Caelo	Wax, bleached	15292002	1
Caelo	Wax, bleached	16163105	21
Caelo	Wax, bleached	15292011	1
Euro OTC	Wax, bleached	16163104	1
Caelo	Wax, bleached	16163109	10
Caelo	Wax, bleached	13378640	2
Caelo	Wax, bleached	16163106	1
phönix	Wax, bleached	15292022	1
phönix	Wax, bleached	16163109	1
Caelo	Wax, bleached	16163114	9
Sanacorp	Wax, bleached	16163114	1
Spinnrad	Wax, bleached	317048061	1
Caelo	Wax, bleached	16163115	2
GEHE	Wax, bleached	16163109	1
Bombastus	Wax, bleached	16163109	1
Noweda	Wax, bleached	16163114	1
Caelo	Wax, bleached	17091802	9
Caelo	Wax, bleached	17091803	2
Bombastus	Wax, bleached	280A171019	1
Spinnrad	Wax, bleached	118048061	1
Klenk	Wax, bleached	280A171019	2
Caelo	Wax, bleached	3051808	1
Caelo	Wax, bleached	18048901	7
Caelo	Wax, bleached	29091805	1
Caelo	Wax, bleached	18048903	2
Caelo	Wax, bleached	18048906	5
Caelo	Wax, bleached	18048907	1
Kehr	Wax, bleached	18048906	1
Caesar & Loretz GmbH	Wax, bleached	18239104	1
Caelo	Cocoa butter	11034718	1
Caelo	Cocoa butter	103276705	1
Caelo	Cocoa butter	11034719	1
Caelo	Cocoa butter	12040803	1
Caelo	Cocoa butter	12040802	1
Caelo	Cocoa butter	11117816	1
Anzag	Cocoa butter	11117816	1
Caelo	Cocoa butter	12040807	2
Caelo	Cocoa butter	12270201	2

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Supplier	Substance	Batch	Spectra
Caelo	Cocoa butter	12342003	7
Caelo	Cocoa butter	12270202	4
Spinnrad	Cocoa butter	512300202	1
Anzag	Cocoa butter	12342004	1
Caelo	Cocoa butter	12270203	4
Caelo	Cocoa butter	13027204	4
Noweda	Cocoa butter	11117813	2
Caelo	Cocoa butter	12342004	1
Caelo	Cocoa butter	13027202	4
Caelo	Cocoa butter	13027203	1
Caelo	Cocoa butter	13027207	1
Sanacorp	Cocoa butter	13027207	1
Caelo	Cocoa butter	13027221	4
Caesar & Loretz GmbH	Cocoa butter	12270210	2
Caelo	Cocoa butter	13027224	4
Sanacorp	Cocoa butter	AKD27	1
Caelo	Cocoa butter	13027226	4
Caelo	Cocoa butter	12270210	1
Caelo	Cocoa butter	13140401	1
Caelo	Cocoa butter	12270209	1
Caelo	Cocoa butter	13140404	2
Caelo	Cocoa butter	13027227	3
Caelo	Cocoa butter	13292006	4
Caelo	Cocoa butter	13292007	9
Caesar & Lorenz	Cocoa butter	13140404	1
Caelo	Cocoa butter	13140405	3
Caelo	Cocoa butter	13292011	2
Caelo / Noweda	Cocoa butter	13292011	1
Caelo	Cocoa butter	13140407	3
Caelo	Cocoa butter	13140406	3
Caelo	Cocoa butter	13292001	2
Caelo	Cocoa butter	13292012	3
Caelo	Cocoa butter	13292013	9
Gutenberg-Apotheke	Cocoa butter	13292007	1
Caelo	Cocoa butter	13292015	1
Sanacorp	Cocoa butter	AKD28	1
Caelo	Cocoa butter	1392013	1
Caelo	Cocoa butter	13292019	3
sanacorp	Cocoa butter	13140407	1
Caelo	Cocoa butter	14123611	6
Caelo	Cocoa butter	13140409	1
Caelo	Cocoa butter	14123617	3
Caelo	Cocoa butter	14123609	1
Caelo	Cocoa butter	14045104	1
Caelo	Cocoa butter	14304703	1
Caelo	Cocoa butter	14123620	5
Caelo	Cocoa butter	14123621	1
Caelo	Cocoa butter	14348906	6
Caelo	Cocoa butter	15088904	1
Caelo	Cocoa butter	14348908	2
Caelo	Cocoa butter	515A-03176	1
ACM	Cocoa butter	KNC1605J15	1
Phönix	Cocoa butter	27121	1
Caelo	Cocoa butter	15088903	1
Caelo	Cocoa butter	15246102	3
AHD	Cocoa butter	14348906	1
Caelo	Cocoa butter	14348909	2
Caelo	Cocoa butter	16049209	2
Caelo	Cocoa butter	16049201	1
Caelo	Cocoa butter	16316501	3

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Supplier	Substance	Batch	Spectra
Caelo	Cocoa butter	16316508	17
Caelo	Cocoa butter	16316503	6
Caelo	Cocoa butter	16316509	4
Caelo	Cocoa butter	163116508	1
Caelo	Cocoa butter	17055902	8
Sanacorp	Cocoa butter	17055908	3
Caelo	Cocoa butter	17055907	10
Caelo	Cocoa butter	17055905	1
Sanacorp	Cocoa butter	170559908	1
Caelo	Cocoa butter	170555901	1
Caelo	Cocoa butter	17055913	1
Spinnrad	Cocoa butter	1017300203	1
Caelo	Cocoa butter	17314902	8
Bombastus	Cocoa butter	17314901	1
Caelo	Cocoa butter	17055908	1
Caelo	Cocoa butter	18135102	1
Sanacorp	Cocoa butter	17314902	1
Sanacorp	Cocoa butter	18135106	3
Caelo	Cocoa butter	18135106	1
Caelo	Hard fat in pastilles	11109623	2
Caelo	Hard fat in pastilles	11109617	1
Caelo	Hard fat in pastilles	11345905	3
Caesar&Loretz GmbH D-40...	Hard fat in pastilles	11109617	1
Caelo	Hard fat in pastilles		1
Noweda	Hard fat in pastilles	11345909	1
Caelo	Hard fat in pastilles	12111204	1
Caelo	Hard fat in pastilles	11345918	7
Fargon	Hard fat in pastilles	41319264	1
Caelo	Hard fat in pastilles	11345904	1
Caelo	Hard fat in pastilles	24011302	1
Caelo	Hard fat in pastilles	12158104	4
Caesar & Loretz GmbH, 4...	Hard fat in pastilles	11345918	1
Caelo	Hard fat in pastilles	1135917	1
Caelo	Hard fat in pastilles	11345917	3
Caelo	Hard fat in pastilles	10158813	1
Caesar & Loretz GmbH D-...	Hard fat in pastilles	12158104	1
Purren Apotheke	Hard fat in pastilles	10I03-N08	1
Fargon	Hard fat in pastilles	12I04-N11	1
Caelo	Hard fat in pastilles	12158109	3
Bombastus	Hard fat in pastilles	273759	1
Fargon	Hard fat in pastilles	12158115	2
Caelo	Hard fat in pastilles	12158115	6
Gehe	Hard fat in pastilles	11345918	1
Caelo	Hard fat in pastilles	12158114	3
Fargon	Hard fat in pastilles	12K01-N12	1
Caelo	Hard fat in pastilles	7101304	1
Caelo	Hard fat in pastilles	13243301	5
Fargon	Hard fat in pastilles	13D10-N06	1
Caelo	Hard fat in pastilles	12158122	1
Gehe	Hard fat in pastilles	13243403	1
AHD	Hard fat in pastilles	277212	2
Caelo	Hard fat in pastilles	13243403	7
Caesar & Loretz GmbH, 4...	Hard fat in pastilles	13243403	1
Caelo	Hard fat in pastilles	90915429	1
Phönix	Hard fat in pastilles	277212	1
Caelo	Hard fat in pastilles	13243416	1
Caelo	Hard fat in pastilles	13243414	1
Phytocomm	Hard fat in pastilles	209314	1
Caelo	Hard fat in pastilles	13243411	3
Caelo	Hard fat in pastilles	13243409	5

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Supplier	Substance	Batch	Spectra
China Medica	Hard fat in pastilles	3244303	1
Caelo	Hard fat in pastilles	14126203	7
Caelo	Hard fat in pastilles	13243412	2
Caelo	Hard fat in pastilles	13243420	1
Fagron	Hard fat in pastilles	12G04-N18	1
Caelo	Hard fat in pastilles	13243418	3
Caelo	Hard fat in pastilles	17041401	1
Caelo	Hard fat in pastilles	13243419	3
Caelo	Hard fat in pastilles	14126205	1
Caelo	Hard fat in pastilles	14126204	2
Caelo	Hard fat in pastilles	12158119	1
Sanacorp	Hard fat in pastilles	14126203	1
Bombastus	Hard fat in pastilles	287287	1
Caelo	Hard fat in pastilles	14126202	4
Fagron	Hard fat in pastilles	13243301	1
Caelo	Hard fat in pastilles	1412602	1
Caelo	Hard fat in pastilles	15111402	1
Caesar/Noweda	Hard fat in pastilles	14126203	1
Caelo	Hard fat in pastilles	14126210	3
Fagron	Hard fat in pastilles	14G03-B03-296731	1
Caelo	Hard fat in pastilles	14126216	2
Caelo	Hard fat in pastilles	14126217	3
Caelo	Hard fat in pastilles	16021503	1
Caelo	Hard fat in pastilles	14126218	2
Caelo	Hard fat in pastilles	14338703	3
Fagron	Hard fat in pastilles	14L01-B06	2
Caelo	Hard fat in pastilles	14338707	3
Bombastus	Hard fat in pastilles	293848	6
Caelo	Hard fat in pastilles	14338705	1
Caelo	Hard fat in pastilles	14338704	4
Caelo	Hard fat in pastilles	20071501	1
Caelo	Hard fat in pastilles	14338711	2
Fagron	Hard fat in pastilles	15F03-B06	4
Fagron	Hard fat in pastilles	14L01-B06-303380	3
Fagron	Hard fat in pastilles	15F03-B06-308708	3
Caelo	Hard fat in pastilles	14338708	1
sanacorp	Hard fat in pastilles	14338703	1
Caelo	Hard fat in pastilles	15185002	11
Cae4lo	Hard fat in pastilles	15185002	1
Caelo	Hard fat in pastilles	14338706	1
Caelo	Hard fat in pastilles	15185003	10
Caelo	Hard fat in pastilles	15185005	12
Rondell Apotheke	Hard fat in pastilles	15185002	1
Caelo	Hard fat in pastilles	15185009	6
Caelo	Hard fat in pastilles	1518505	1
Euro OTC	Hard fat in pastilles	15185005	1
Caelo	Hard fat in pastilles	16027801	4
Caelo	Hard fat in pastilles	16027802	7
Caelo	Hard fat in pastilles	16274201	8
Bombastus	Hard fat in pastilles	302709	1
Caelo	Hard fat in pastilles	15185007	1
Caelo	Hard fat in pastilles	16274205	3
Caelo	Hard fat in pastilles	16274203	7
Caelo	Hard fat in pastilles	8041710	1
Sanacorp	Hard fat in pastilles	16274202	1
Bombastus	Hard fat in pastilles	306363	4
Caelo	Hard fat in pastilles	16274202	1
GEHE	Hard fat in pastilles	16274203	1
Phönix	Hard fat in pastilles	16274203	1
Caelo	Hard fat in pastilles	170921AS/16274208	1

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Supplier	Substance	Batch	Spectra
Caelo	Hard fat in pastilles	17107301	5
Caelo	Hard fat in pastilles	16274208	3
Caelo	Hard fat in pastilles	27101703	1
Euro OTC	Hard fat in pastilles	17107304	1
Caelo	Hard fat in pastilles	17107306	2
Bombastus	Hard fat in pastilles	308559	1
Bombastus	Hard fat in pastilles	17107304	1
Caelo	Hard fat in pastilles	17107304	1
Caelo	Hard fat in pastilles	17307602	5
Caelo	Hard fat in pastilles	17307601	11
Caelo	Hard fat in pastilles	8051810	1
Bombastus	Hard fat in pastilles	18000346	3
Caelo	Hard fat in pastilles	17307604	1
Caelo	Hard fat in pastilles	29061803	1
Caelo	Hard fat in pastilles	18147901	2
Caelo	Sodium dodecyl sulfate	11220208	1
Caelo	Sodium dodecyl sulfate	12153003	1
Caelo	Sodium dodecyl sulfate	12153010	3
Caelo	Sodium dodecyl sulfate	12153004	1
Caelo	Sodium dodecyl sulfate	12153019	1
Caelo	Sodium dodecyl sulfate	13014604	2
Caelo	Sodium dodecyl sulfate	13099006	3
Caelo	Sodium dodecyl sulfate	13099011	3
Sanacorp	Sodium dodecyl sulfate	5/AKD1	1
Caelo	Sodium dodecyl sulfate	13411302	2
Caelo	Sodium dodecyl sulfate	13411305	3
Gehe	Sodium dodecyl sulfate	14127404	1
Caelo	Sodium dodecyl sulfate	13411304	1
Caelo	Sodium dodecyl sulfate	14127406	1
Caelo	Sodium dodecyl sulfate	14127411	1
Caelo	Sodium dodecyl sulfate	14283904	3
Caelo	Sodium dodecyl sulfate	26031508	1
Caelo	Sodium dodecyl sulfate	14224206	1
Sanacorp	Sodium dodecyl sulfate	5/AKD6	1
Caelo	Sodium dodecyl sulfate	15095404	1
Caelo	Sodium dodecyl sulfate	15119907	3
Caelo	Sodium dodecyl sulfate	15344503	3
Caelo	Sodium dodecyl sulfate	15344505	2
Caelo	Sodium dodecyl sulfate	15344511	1
Ichthyol/Phönix	Sodium dodecyl sulfate	15344510	1
Caelo	Sodium dodecyl sulfate	15344515	2
Caelo	Sodium dodecyl sulfate	15344510	4
Caelo	Sodium dodecyl sulfate	16229206	4
Fagron	Sodium dodecyl sulfate	16229205	1
GEHE	Sodium dodecyl sulfate	16229205	1
Intern Drogen	Sodium dodecyl sulfate	216991080	1
Caelo	Sodium dodecyl sulfate	16229217	2
Caelo	Sodium dodecyl sulfate	16229213	2
Caelo	Sodium dodecyl sulfate	16229218	1
Caelo	Sodium dodecyl sulfate	16229209	1
Caelo	Sodium dodecyl sulfate	16229205	2
Caelo	Sodium dodecyl sulfate	16229220	1
Caelo	Sodium dodecyl sulfate	17095504	1
Caelo	Sodium dodecyl sulfate	17095511	2
Caesar & Loretz GmbH	Sodium dodecyl sulfate	17095504	1
Caelo	Paraffin, microcrystalline	30101202	1
Caelo	Paraffin, microcrystalline	7111201	1
Caelo	Paraffin, microcrystalline	12095101	1
Caelo	Paraffin, microcrystalline	7111202	1
Noweda	Paraffin, microcrystalline	12266304	1

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin, microcrystalline	3042012M1	1
Caelo	Paraffin, microcrystalline	12355001	1
Caelo	Paraffin, microcrystalline	13274303	5
Caelo	Paraffin, microcrystalline	13274301	1
Phönix	Paraffin, microcrystalline	13274301	1
Caelo	Paraffin, microcrystalline	14307110	1
Caelo	Paraffin, microcrystalline	14307108	2
Caelo	Paraffin, microcrystalline	52622395	1
Caelo	Paraffin, microcrystalline	15412801	2
Caelo	Paraffin, microcrystalline	15412808	1
Caelo	Paraffin, microcrystalline	17137502	1
Noweda	Paraffin, hard	11363206	1
Caelo	Paraffin, hard	1136206	1
Caelo	Paraffin, hard	12252205	2
Caelo	Paraffin, hard	11363220	3
Caelo	Paraffin, hard	11363206	2
Caelo	Paraffin, hard	11363205	1
Caelo	Paraffin, hard	10194101	2
Caelo	Paraffin, hard	12252211	3
Caelo	Paraffin, hard	12252221	3
Caelo	Paraffin, hard	13109203	4
Caelo	Paraffin, hard	13109213	6
Caelo	Paraffin, hard	12252206	1
Caelo	Paraffin, hard	13109214	4
Caelo	Paraffin, hard	11021202	1
Caelo	Paraffin, hard	13109221	1
Caelo	Paraffin, hard	13109218	1
Caelo	Paraffin, hard	13109224	4
Unisan	Paraffin, hard	11166911	3
Caelo	Paraffin, hard	13390406	4
Caelo	Paraffin, hard	13390413	1
Caelo	Paraffin, hard	13390403	1
Caelo	Paraffin, hard	14126202	1
Euro OTC	Paraffin, hard	13109224	1
Caelo	Paraffin, hard	14286503	1
Caelo	Paraffin, hard	14286504	1
Caelo	Paraffin, hard	13390415	2
Caelo	Paraffin, hard	14286502	1
Phoenix goettingen 09.05	Paraffin, hard	13390415	1
Caelo	Paraffin, hard	14286517	4
Caelo	Paraffin, hard	14286511	2
Caelo	Paraffin, hard	123654	1
Caelo	Paraffin, hard	13390408	1
Caelo	Paraffin, hard	1523002	1
Bombastus	Paraffin, hard	293848	1
Noweda	Paraffin, hard	14286517	1
Caelo	Paraffin, hard	15232004	5
Caelo	Paraffin, hard	152320004	1
Caelo	Paraffin, hard	15295405	5
Caelo	Paraffin, hard	15232001	1
Caelo	Paraffin, hard	15295406	2
Caelo	Paraffin, hard	15295410	2
Phoenix	Paraffin, hard	15295410	1
Cealo/AHD	Paraffin, hard	15295411	2
Caelo	Paraffin, hard	15295414	3
Caelo	Paraffin, hard	15295407	1
Caelo	Paraffin, hard	16000903	2
GEHE	Paraffin, hard	15295409	1
Caelo	Paraffin, hard	302709	1
Caelo	Paraffin, hard	16000922	3

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin, hard	16000912	2
Caelo	Paraffin, hard	16000911	2
Caelo	Paraffin, hard	16000921	1
Caelo	Paraffin, hard	16000910	1
Gehe	Paraffin, hard	15295410	1
Caelo	Paraffin, hard	16277704	2
HCK	Paraffin, hard	16277705	1
Caelo	Paraffin, hard	16277705	2
Caelo	Paraffin, hard	16277710	2
Caelo	Paraffin, hard	16277706	2
Caelo	Paraffin, hard	17245602	5
Caelo	Paraffin, hard	17107304	1
Caelo	Paraffin, hard	17347701	4
Jenne	Paraffin, hard	17347701	1
Kehr	Paraffin, hard	17347701	1
Caelo	Paraffin, hard	18070107	2
Caesar & Loretz	Paraffin, hard	18070107	1
Caelo	Cetyl palmitate 15	26071201	1
Caelo	Cetyl palmitate 15	12018204	3
Caelo	Cetyl palmitate 15	12082901	1
Caesar & Loretz GmbH	Cetyl palmitate 15	10068402	2
Caelo	Cetyl palmitate 15	12018208	6
Caelo	Cetyl palmitate 15	12018215	1
Anzag	Cetyl palmitate 15	12018208	1
Caelo	Cetyl palmitate 15	11042019	1
Caelo	Cetyl palmitate 15	12228808	3
Fagron	Cetyl palmitate 15	12C27-N07	2
Gehe	Cetyl palmitate 15	8209646	1
Caelo	Cetyl palmitate 15	12228808	1
Caesar/Noweda	Cetyl palmitate 15	12228801	1
Euro OTC	Cetyl palmitate 15	12228808	1
Caelo	Cetyl palmitate 15	12228805	1
Caelo	Cetyl palmitate 15	12228818	5
Caelo	Cetyl palmitate 15	12331916	8
Caelo	Cetyl palmitate 15	12331919	2
Fagron	Cetyl palmitate 15	12D19-N02	1
Caelo	Cetyl palmitate 15	13131905	3
Alliance Healthcare	Cetyl palmitate 15	13131905	1
Caelo	Cetyl palmitate 15	12018204/Int212191	1
Caelo	Cetyl palmitate 15	122228801/Int212191	1
Caelo	Cetyl palmitate 15	13131911	2
Caelo	Cetyl palmitate 15	13131906	6
Nachprüfung	Cetyl palmitate 15	3012U01241	1
Caelo	Cetyl palmitate 15	30101301	1
Caelo	Cetyl palmitate 15	10068410	1
Sanacorp	Cetyl palmitate 15	8/AKD12	1
Caelo	Cetyl palmitate 15	1313190	1
Caelo	Cetyl palmitate 15	13131914	4
Phönix	Cetyl palmitate 15	13131906	1
Caelo	Cetyl palmitate 15	13295910	8
Caelo	Cetyl palmitate 15	13295919	10
Phönix	Cetyl palmitate 15	13295919	1
Caelo	Cetyl palmitate 15	14060705	6
Caelo	Cetyl palmitate 15	14060709	6
Caelo	Cetyl palmitate 15	14060706	6
Phoenix	Cetyl palmitate 15	14060705	1
Caelo	Cetyl palmitate 15	13295921	1
Caesar/Noweda	Cetyl palmitate 15	13295909	1
Caelo	Cetyl palmitate 15	14213705	3
Caelo	Cetyl palmitate 15	14213709	4

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Supplier	Substance	Batch	Spectra
Caelo	Cetyl palmitate 15	11021502	1
Sanacorp	Cetyl palmitate 15	8/AKD13	1
Caesar u Loretz	Cetyl palmitate 15	14213710	1
Caelo	Cetyl palmitate 15	14213710	2
Caelo	Cetyl palmitate 15	14041505	1
Caelo	Cetyl palmitate 15	14351602	4
Caelo	Cetyl palmitate 15	14351601	2
Caelo	Cetyl palmitate 15	14351612	14
Caelo	Cetyl palmitate 15	14351606	4
Caelo	Cetyl palmitate 15	14213706	1
Fargon/Alliance HC	Cetyl palmitate 15	14351612	1
Caelo	Cetyl palmitate 15	14351609	3
Caelo	Cetyl palmitate 15	15301703	7
Caelo	Cetyl palmitate 15	142137710	1
coelo/Sana	Cetyl palmitate 15	14351612	1
Caelo	Cetyl palmitate 15	14351614	1
Caelo	Cetyl palmitate 15	15301704	5
Caelo	Cetyl palmitate 15	15301701	5
Caelo	Cetyl palmitate 15	15301709	5
Caelo	Cetyl palmitate 15	14351607	1
Caelo	Cetyl palmitate 15	15632	1
Caesar/Noweda	Cetyl palmitate 15	15301701	1
Caelo	Cetyl palmitate 15	15301705	6
Caelo	Cetyl palmitate 15	16053803	9
Alliance H.	Cetyl palmitate 15	15301709	1
Caelo	Cetyl palmitate 15	16053805	2
Caelo	Cetyl palmitate 15	15301711	4
Caelo	Cetyl palmitate 15		2
Euro OTC	Cetyl palmitate 15	160419C	1
Caelo	Cetyl palmitate 15	16053804	1
Fischer/Phönix	Cetyl palmitate 15	15301711	1
Caelo	Cetyl palmitate 15	16053811	6
Caelo	Cetyl palmitate 15	16186805	15
Caelo	Cetyl palmitate 15	16186809	6
Sanacorp	Cetyl palmitate 15	16186805	1
Caesar & Loretz GmbH	Cetyl palmitate 15	16186805	1
Caelo	Cetyl palmitate 15	28041731	1
Caelo	Cetyl palmitate 15	16186806	1
Caelo	Cetyl palmitate 15	17043503	4
Caelo	Cetyl palmitate 15	17043504	5
Caelo	Cetyl palmitate 15	17164005	9
Caelo	Cetyl palmitate 15	17164004	6
Caelo	Cetyl palmitate 15	17164007	1
Caesar & Lorenz GmbH	Cetyl palmitate 15	17043504	1
Caelo	Cetyl palmitate 15	17043509	1
Caelo	Cetyl palmitate 15	17271506	1
Caelo	Cetyl palmitate 15	17271505	3
Caesar & Loretz GmbH	Cetyl palmitate 15	17164005	1
Caelo	Cetyl palmitate 15	17271502	4
Caelo	Cetyl palmitate 15	17271504	3
Fargon	Cetyl palmitate 15	17164005	1
Caelo	Cetyl palmitate 15	18149904	1
Caelo	Cetyl palmitate 15	19121803	1
Caesar & Loretz GmbH	Cetyl palmitate 15	18149912	1
Fargon	Hard fat W35	15J08-B04-322726	1
Noweda	Hard fat W35	16027801	1
Fargon	Hard fat W35	3914E-02328	1
Bombastus	Hard fat W35	302709	2
Phoenix	Hard fat W35	16k08-b10-332763	1
Fargon	Hard fat W35	15J08-B04-324959	2

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Supplier	Substance	Batch	Spectra
Fagron	Hard fat W35	15A07-B12-309245	1
Fagron	Hard fat W35	16K08-B10-332763	1
Fagron	Hard fat W35	17K09-B03-346709	1
Fagron	Hard fat W35	17k09-b03-351980	1
Kehr	Hard fat W35	17K09-B03-351980	1

- 77 030 spectra from 565 *Apo-Ident* customers from a total of 25 520 batches from a further 685 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Waxes / Fats* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Waxes / Fats* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	1207	0	73 289
Type B	0	1386	7	125 499
Type C	0	1843	56	77 030

The substance/substance group *Waxes / Fats* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 99.5029 %)
Type B	100.0000 % (> 99.9901 %)	99.4975 % (> 99.2821 %)
Type C	100.0000 % (> 99.8817 %)	97.0511 % (> 96.8931 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
20865	20865	0.00	33.40
21875	21984	4.88	27.71
21984	21984	0.00	30.08
22325	21984	2.73	28.96
22486	22486	0.00	28.82
21067	22479	6.29	48.63
22479	22479	0.00	46.17
23565	22479	18.26	53.42
21433	22767	7.31	28.17
22245	22767	4.72	26.00
22767	22767	0.00	22.56
20747	22767	11.00	32.98
22244	22767	10.23	29.71
22956	22767	12.84	28.45
22349	22349	0.00	26.45
22352	23278	6.57	38.66
23242	20986	6.55	40.06
23278	23278	0.00	36.16
21682	21682	0.00	20.69
21766	22330	2.50	21.73
21482	23067	13.58	72.40
22330	22330	0.00	22.20
21880	21880	0.00	42.64
22348	23067	4.59	61.96
22338	21880	5.13	43.15
23067	23067	0.00	58.79
23601	21880	2.34	39.99
23707	23067	3.99	64.02
21483	21483	0.00	20.27
20986	20986	0.00	41.76
21731	22349	1.96	26.26

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Wool alcohols**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20495-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Wool alcohols; Alcoholes lanae

Special notes

When selecting the *Wool alcohols* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 alcohols*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Wool alcohols	13380601	21520	40	1412037
Caelo	Wool alcohols	153703	22328	40	20151111*
Caelo	Wool alcohols	153703	22329	40	20151111*

Validation samples

A total of 280 317 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 *Wool alcohols*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1621 batches from further 372 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 *Wool alcohols*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Wool alcohols	153703	22328 [†]	20
Caelo	Wool alcohols	153703	22329 [†]	20
Caelo	Wool alcohols	163530	23098	40
Caelo	Wool alcohols	173160	23972	40
Caelo	Wool alcohols	181619	24165	40

- 126 732 spectra from a total of 2785 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 20 spectra from 11 *Apo-Ident* customers from 15 batches from the substance/substance group *Wool alcohols*.

*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	Wool alcohols	13083906	2
Caelo	Wool alcohols	12340505	1
Caelo	Wool alcohols	13083912	1
Caelo	Wool alcohols	11011401	1
Cealo/ Noweda	Wool alcohols	13380601	1
Caelo	Wool alcohols	13380601	1
Caelo	Wool alcohols	13226408	1
Caelo	Wool alcohols	4/2015	1
Caelo	Wool alcohols	23101408	1
Caelo	Wool alcohols	14262501	1
Caelo	Wool alcohols	13071502	1
Caelo	Wool alcohols	15304502	1
Caelo	Wool alcohols	15304505	2
Caelo	Wool alcohols	17169701	3
Fagron	Wool alcohols	16235702	1
Caelo	Wool alcohols	6111801	1

- 78 909 spectra from 565 *Apo-Ident* customers from a total of 26 122 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 alcohols* can clearly be 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 alcohols* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	160	0	126 732
Type C	0	19	1	78 909

The substance/substance group *Wool alcohols* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.8817 %)	95.0000 % (> 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
21520	21520	0.00	54.80
22328	22328	0.00	43.50
22329	22329	0.00	43.55

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Xylitol**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20994-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Xylitol; Xylitolum

Special notes

When selecting the *Xylitol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Xylitol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Xylitol	14G04-B04-298356	21754	40	AR-15-FG-008046-01
Caelo	Xylitol	14068206	21755	40	20140317
Caelo	Xylitol	15135405	22248	40	20150417
Fagron	Xylitol	14G04-B04-303524	22254	40	20140919

Validation samples

A total of 280 317 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 *Xylitol*. These samples are listed above in the [calibration samples](#) section.
- 74 336 spectra from a total of 1619 batches from further 372 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 8 reference samples from the substance/substance group *Xylitol*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Xylitol	14G04-B04-298356	21754 [†]	20
Caelo	Xylitol	14068206	21755 [†]	20
Caelo	Xylitol	15135405	22248 [†]	20
Fagron	Xylitol	14G04-B04-303524	22254 [†]	20
Caelo	Xylitol	15388101	22578	40
Caelo	Xylitol	15135405	22579	40
Caelo	Xylitol	163174	23061	40
Caelo	Xylitol	181133	24041	40

- 126 652 spectra from a total of 2782 batches from further 781 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*.

- 26 spectra from 12 *Apo-Ident* customers from 19 batches from the substance/substance group *Xylitol*.

Supplier	Substance	Batch	Spectra
Fagron	Xylitol	13H28-N10	2
Caelo	Xylitol	5112I-02787	1
Caelo	Xylitol	13230305	1
Caelo	Xylitol	13230302	1
Caelo	Xylitol	13230309	1
Caelo	Xylitol	12240612	1
Caelo	Xylitol	14061401	1
Fagron	Xylitol	13/23-N06	1
Caelo	Xylitol	13230315	1
Fagron	Xylitol	13H28N10	1
Caelo	Xylitol	14G04-B04-298356	2
Caelo	Xylitol	14068206	1
Fagron	Xylitol	14G04-B04-303524	2
Caelo	Xylitol	3314M-02787	1
Fagron	Xylitol	12J25-N06	2
Caelo	Xylitol	15388104	2
Fagron	Xylitol	16c14-B02-320887	1
Caelo	Xylitol	18045302	3
Caelo	Xylitol	18113304	1

- 78 903 spectra from 565 *Apo-Ident* customers from a total of 26 118 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Xylitol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xylitol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	240	0	126 652
Type C	0	26	0	78 903

The substance/substance group *Xylitol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.8817 %)	100.0000 % (> 76.9231 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
21754	21754	0.00	28.53
21755	21754	8.06	39.63
22248	21754	8.55	39.64
22254	21754	2.30	27.97

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Xylometazoline hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20025-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Xylometazoline hydrochloride; Xylometazolini hydrochloridum

Special notes

When selecting the *Xylometazoline hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Xylometazoline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Xylometazoline h...	13344901	21516	40	1501655
Fagron	Xylometazoline h...	13I18-B03-295481	21722	40	AR-15-FG-007785-01
Fagron	Xylometazoline h...	14K19-B05-305006	21927	40	20141128
Caelo	Xylometazoline h...	16074211	23246	40	20160318
Fagron	Xylometazoline h...	14K19-B05-305006	21927SI	40	20141128

Validation samples

A total of 280317 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 *Xylometazoline hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74296 spectra from a total of 1619 batches from further 372 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 [†].

- 480 spectra of 13 reference samples from the substance/substance group *Xylometazoline hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Xylometazoline hydrochloride	13344901	21516 [†]	20
Caelo	Xylometazoline hydrochloride	13344901	21517	60
Fagron	Xylometazoline hydrochloride	13I18-B03-295481	21722 [†]	20
Fagron	Xylometazoline hydrochloride	14K19-B05-305006	21927 [†]	20
Caelo	Xylometazoline hydrochloride	170739	23314	40
Caelo	Xylometazoline hydrochloride	170739	23320	40
Caelo	Xylometazoline hydrochloride	173457	23832	40
Caelo	Xylometazoline hydrochloride	13344901	21517SI	60
Fagron	Xylometazoline hydrochloride	14K19-B05-305006	21927SI [†]	20
Caelo	Xylometazoline hydrochloride	16074211	23246SI	40
Caelo	Xylometazoline hydrochloride	170739	23314SI	40
Caelo	Xylometazoline hydrochloride	170739	23320SI	40
Caelo	Xylometazoline hydrochloride	173457	23832SI	40

- 126412 spectra from a total of 2783 batches from further 781 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](#).

[†]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.

- 109 spectra from 75 *Apo-Ident* customers from 51 batches from the substance/substance group *Xylometazoline hydrochloride*.

Supplier	Substance	Batch	Spectra
Caelo	Xylometazoline hydrochloride	10118821	2
Caelo	Xylometazoline hydrochloride	24111202	1
Noweda	Xylometazoline hydrochloride	12027902	1
Sanacorp	Xylometazoline hydrochloride	12027902	1
Fagron	Xylometazoline hydrochloride	12G31-N01	1
Caelo	Xylometazoline hydrochloride	12027906	2
Caelo	Xylometazoline hydrochloride	12287201	2
Caelo	Xylometazoline hydrochloride	9276404	1
Gehe	Xylometazoline hydrochloride	10118802	1
Caelo	Xylometazoline hydrochloride	12287203	8
Noweda	Xylometazoline hydrochloride	12287203	1
Anzag	Xylometazoline hydrochloride	12027911	1
Caelo	Xylometazoline hydrochloride	12287210	7
Fagron	Xylometazoline hydrochloride	12287210	1
Caelo	Xylometazoline hydrochloride	12287204	2
Caelo	Xylometazoline hydrochloride	9278404	1
Caelo	Xylometazoline hydrochloride	13171202	10
Caelo	Xylometazoline hydrochloride	13171203	2
Caelo	Xylometazoline hydrochloride	12287212	2
Caelo	Xylometazoline hydrochloride	12287213	1
Fagron	Xylometazoline hydrochloride	13E06-N11	1
Fagron	Xylometazoline hydrochloride	13171203	1
Fagron	Xylometazoline hydrochloride	13I09-N02	1
Celoa vdL	Xylometazoline hydrochloride	13171202	1
Caelo	Xylometazoline hydrochloride	13344901	1
Caelo	Xylometazoline hydrochloride	13344908	1
Caelo	Xylometazoline hydrochloride	2031502	1
Caelo	Xylometazoline hydrochloride	13171205	1
Fagron	Xylometazoline hydrochloride	1318-B03-295479	1
Caelo	Xylometazoline hydrochloride	15037907	3
Caelo	Xylometazoline hydrochloride	153037907	1
Sanacorp	Xylometazoline hydrochloride	15037906	1
Anzag	Xylometazoline hydrochloride	15037907	2
Caelo	Xylometazoline hydrochloride	15037906	1
Caelo	Xylometazoline hydrochloride	15037910	2
Caelo	Xylometazoline hydrochloride	15292803	3
Caelo	Xylometazoline hydrochloride	15292804	4
Caelo	Xylometazoline hydrochloride	15037912	1
Caelo	Xylometazoline hydrochloride	16074201	3
Caelo	Xylometazoline hydrochloride	15292811	1
Caelo	Xylometazoline hydrochloride	15292812	2
Fagron	Xylometazoline hydrochloride	10416XMH	1
Caelo	Xylometazoline hydrochloride	16074205	4
Caelo	Xylometazoline hydrochloride	16074216	2
GEHE	Xylometazoline hydrochloride	16074209	1
Caelo	Xylometazoline hydrochloride	16074209	1
Caelo	Xylometazoline hydrochloride	160740209	1
Caelo	Xylometazoline hydrochloride	16074217	2
Caelo	Xylometazoline hydrochloride	16074202	1
Caelo	Xylometazoline hydrochloride	160742095416	1
Caelo	Xylometazoline hydrochloride	1703902	1
Caelo	Xylometazoline hydrochloride	17073902	1

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Supplier	Substance	Batch	Spectra
Caelo	Xylometazoline hydrochloride	17073909	1
Caelo	Xylometazoline hydrochloride	17073905	5
Caelo	Xylometazoline hydrochloride	23051820	1
Caelo	Xylometazoline hydrochloride	17345703	1
Caelo	Xylometazoline hydrochloride	17345707	1
Caelo	Xylometazoline hydrochloride	17345706	1
Sanacorp	Xylometazoline hydrochloride	17345703	1
Caelo	Xylometazoline hydrochloride	17345708	1

- 78 820 spectra from 565 *Apo-Ident* customers from a total of 26 086 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Xylometazoline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xylometazoline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 296
Type B	0	475	5	126 412
Type C	0	89	20	78 820

The substance/substance group *Xylometazoline hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9901 %)	98.9583 % (> 98.3333 %)
Type C	100.0000 % (> 99.8817 %)	81.6514 % (> 78.8991 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower 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
21516	21516	0.00	41.85
21722	21722	0.00	51.42
21927	21722	4.55	51.83
23246	21722	5.36	51.47

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Xylose**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20517-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Xylose; Xylosum

Special notes

When selecting the *Xylose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Xylose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Xylose	14218902	21606	40	AR-14-FG-013086-01
Fagron	Xylose	13A31-B40-292395	21763	40	20140407
Caelo	Xylose	17160902	23413	40	20170704

Validation samples

A total of 280 317 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 *Xylose*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 7 reference samples from the substance/substance group *Xylose*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Xylose	13133402	20868	40
Caelo	Xylose	14218902	21606 [†]	20
Fagron	Xylose	13A31-B40-292395	21763 [†]	20
Caelo	Xylose	162064	22758	40
Fagron	Xylose	16A25-B05-328261	23524	40
Caelo	Xylose	171609	23656	40
Caelo	Xylose	173188	23849	40

- 126 652 spectra from a total of 2782 batches from further 781 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 10 *Apo-Ident* customers from 22 batches from the substance/substance group *Xylose*.

[†]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	Xylose	12120101	1
Caelo	Xylose	13133404	2
Caelo	Xylose	13133414	3
Caelo	Xylose	13133410	1
Falcento	Xylose	2013051801	1
Fagron	Xylose	80414PJK01	1
Eigenherstellung	Xylose	80414HJK01	1
Fagron	Xylose	13133415	1
Phoenix 20.06.2014	Xylose	13A31-B04-292396	1
Fagron	Xylose	28111405	1
Phoenix Goettin	Xylose	13133422	1
Fagron	Xylose	10121401	1
Fagron	Xylose	14E-B03300658	1
Caelo	Xylose	5031501	1
Caelo	Xylose	11031501	1
Caelo	Xylose	16002302	2
Ebert & Jacobi 12.07...	Xylose	16002301	2
Caelo	Xylose	16002301	1
Caelo	Xylose	16002309	1
Caelo	Xylose	16206405	1
Euro OTC	Xylose		1
Caelo	Xylose	17160905	1
Caelo	Xylose	17160902	1

- 78 901 spectra from 565 *Apo-Ident* customers from a total of 26 115 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Xylose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xylose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	240	0	126 652
Type C	0	26	2	78 901

The substance/substance group *Xylose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.8817 %)	92.8571 % (> 82.1429 %)

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
21606	21606	0.00	56.64
21763	21606	14.39	56.83
23413	21606	14.83	56.95

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Zinc acetate dihydrate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20398-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Zinc acetate dihydrate; Zincum aceticum purum

Special notes

When selecting the *Zinc acetate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Zinc acetate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Zinc acetate dihyd...	15383301	22728	40	20151127
Caelo	Zinc acetate dihyd...	153833	23030	40	20151127*
Caelo	Zinc acetate dihyd...	170204	23031	40	20170126*

Validation samples

A total of 280 317 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 *Zinc acetate dihydrate*. These samples are listed above in the [calibration samples](#) section.
- 74 376 spectra from a total of 1620 batches from further 372 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 *Zinc acetate dihydrate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Zinc acetate dihydrate	17020404	23514	40
Caelo	Zinc acetate dihydrate	170204	23637	40
Caelo	Zinc acetate dihydrate	182046	24213	40

- 126 772 spectra from a total of 2786 batches from further 781 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 20 spectra from 18 *Apo-Ident* customers from 13 batches from the substance/substance group *Zinc acetate dihydrate*.

Supplier	Substance	Batch	Spectra
Caelo	Zinc acetate dihydrate	12134803	1

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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
Caelo	Zinc acetate dihydrate	12316401	1
Caelo	Zinc acetate dihydrate	12316403	2
Caelo	Zinc acetate dihydrate	12134801	2
Caelo	Zinc acetate dihydrate	12316404	2
Caelo	Zinc acetate dihydrate	12316405	1
phönix	Zinc acetate dihydrate	15383301	1
Caelo	Zinc acetate dihydrate	15160801	1
Caelo	Zinc acetate dihydrate	15383306	3
Caelo	Zinc acetate dihydrate	15160804	1
Caelo	Zinc acetate dihydrate	17020403	2
Caelo	Zinc acetate dihydrate	17197601	2
Caelo	Zinc acetate dihydrate	15383304	1

- 78 909 spectra from 565 *Apo-Ident* customers from a total of 26 124 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Zinc acetate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zinc acetate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	120	0	126 772
Type C	0	5	15	78 909

The substance/substance group *Zinc acetate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	25.0000 % (> 10.0000 %)

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
22728	23030	3.07	49.26
23030	23030	0.00	50.90
23031	23031	0.00	48.50

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **Zinc gluconate**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20379-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Zinc gluconate; Zincum gluconicum

Special notes

When selecting the *Zinc gluconate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *Zinc gluconate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Zinc gluconate	1407033-02	21709	40	20140902
Euro OTC	Zinc gluconate	1508007	21882	40	20150827*
Euro OTC	Zinc gluconate	1603035	22513	40	20160427*
Caelo	Zinc gluconate	170165	23034	40	20170125*
Caelo	Zinc gluconate	170951	23292	40	20170518*
Euro OTC	Zinc gluconate	1807019	24150	40	20180725*

Validation samples

A total of 280 317 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 *Zinc gluconate*. These samples are listed above in the [calibration samples](#) section.
- 74 256 spectra from a total of 1617 batches from further 372 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 [†].

- 280 spectra of 8 reference samples from the substance/substance group *Zinc gluconate*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Zinc gluconate	1407033-02	21709 [†]	20
Euro OTC	Zinc gluconate	1508007	21882 [†]	20
Caelo	Zinc gluconate	161788	22619	40
Euro OTC	Zinc gluconate	1606018	22700	40
Euro OTC	Zinc gluconate	1701017	22994	40
Euro OTC	Zinc gluconate	1706009	23544	40
Euro OTC	Zinc gluconate	1711004	23730	40
Euro OTC	Zinc gluconate	1810014	24347	40

- 126 612 spectra from a total of 2781 batches from further 781 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.

- 10 spectra from 7 *Apo-Ident* customers from 8 batches from the substance/substance group *Zinc gluconate*.

Supplier	Substance	Batch	Spectra
Euro OTC	Zinc gluconate	1312010-01	1
Euro OTC	Zinc gluconate	1405011-01	1
Fagron	Zinc gluconate	14J30-B06-300520	1
Caelo	Zinc gluconate	16178801	1
Caelo	Zinc gluconate	17016502	2
Euro OTC	Zinc gluconate	27061711	1
Caelo	Zinc gluconate	17095103	1
Euro OTC	Zinc gluconate	1711004-01	2

- 78 919 spectra from 565 *Apo-Ident* customers from a total of 26 129 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Zinc gluconate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zinc gluconate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 256
Type B	0	280	0	126 612
Type C	0	10	0	78 919

The substance/substance group *Zinc gluconate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.8818 %)	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
22513	22513	0.00	26.48
24150	24150	0.00	19.41
21709	23292	5.63	20.67
21882	21882	0.00	24.94
23034	23034	0.00	24.74
23292	23292	0.00	24.27

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **3.4-diaminopyridine**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20317-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

3.4-diaminopyridine; 3,4-Diaminopyridinum

Special notes

When selecting the *3.4-diaminopyridine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *3.4-diaminopyridine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	3.4-diaminopyrid...	13F05-N01	20901	40	20130606
Inresa	3.4-diaminopyrid...	0631350001	21781	40	8899
Fagron	3.4-diaminopyrid...	16A22-B04-317264	22321	40	20160204
Inresa	3.4-diaminopyrid...	33-15-IV-56P2749B	22848	40	20160822

Validation samples

A total of 280317 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 *3,4-diaminopyridine*. These samples are listed above in the [calibration samples](#) section.
- 74336 spectra from a total of 1619 batches from further 372 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 [†].

- 161 spectra of 6 reference samples from the substance/substance group *3,4-diaminopyridine*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	3,4-diaminopyridine	13F05-N01	20901 [†]	1
Inresa	3,4-diaminopyridine	0631350001	21781 [†]	20
Fagron	3,4-diaminopyridine	16A22-B04-317264	22321 [†]	20
Inresa	3,4-diaminopyridine	33-16-I-77P3018	23723	40
Fagron	3,4-diaminopyridine	17J11-B01-340962	23766	40
Caelo	3,4-diaminopyridine	17251208	24177	40

- 126731 spectra from a total of 2783 batches from further 781 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.

- 51 spectra from 9 *Apo-Ident* customers from 25 batches from the substance/substance group *3,4-diaminopyridine*.

[†]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
Fagron	3.4-diaminopyridine	11K07-N02	1
Fagron	3.4-diaminopyridine	11/14-N03	1
Inresa	3.4-diaminopyridine	508670001	1
Caelo	3.4-diaminopyridine	13f05-n01	1
Gehe	3.4-diaminopyridine	13F07-N07	1
Fagron	3.4-diaminopyridine	13F07-N07	1
Inresa	3.4-diaminopyridine	580710001	9
Fagron	3.4-diaminopyridine	13L12-M03	1
Fagron	3.4-diaminopyridine	13K14-M01	1
inresa	3.4-diaminopyridine	58010001	2
Fagron	3.4-diaminopyridine	13L12-M06	2
inresa	3.4-diaminopyridine	58710001	2
Fagron	3.4-diaminopyridine	14H11-B06	3
inresa	3.4-diaminopyridine	580710001	2
Caelo	3.4-diaminopyridine	14H11-B06-298447	2
Inresa	3.4-diaminopyridine	63150001	1
Inresa	3.4-diaminopyridine	631350001	3
Fagron	3.4-diaminopyridine	15B20-B02	2
inresa	3.4-diaminopyridine	631350001	1
Fagron	3.4-diaminopyridine	16D05-B01	1
Inresa	3.4-diaminopyridine	33-15-IV-56P2749	2
Fagron	3.4-diaminopyridine	16D05-B01-318216	1
Inresa	3.4-diaminopyridine	33-15-IV-56P2749B/22	3
Inresa	3.4-diaminopyridine	33-15-IV-56P2749B	2
Inresa	3.4-diaminopyridine	33-16-I-77P3018/1307	1
Fagron	3.4-diaminopyridine	16K15-B03-330546	1
Inresa	3.4-diaminopyridine	33-16-I-77P3018	2
Inresa Arzneimittel GmbH	3.4-diaminopyridine	33-16-I-77P3018/1307	1

- 78 878 spectra from 565 *Apo-Ident* customers from a total of 26 113 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *3.4-diaminopyridine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *3.4-diaminopyridine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 336
Type B	0	161	0	126 731
Type C	0	42	9	78 878

The substance/substance group *3.4-diaminopyridine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 96.2733 %)
Type C	100.0000 % (> 99.8817 %)	82.3529 % (> 76.4706 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower 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
20901	21781	4.35	32.30
21781	21781	0.00	31.92
22321	21781	4.48	31.98
22848	21781	3.17	32.00

VALIDATION REPORT

IdentModul 2.0-2019-02

Validated substance/substance group **5-aminolevulinic acid hydrochloride**
Substance class APIs & excipients, solid
Report date 24/05/2019
Report number 20371-2019-05-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

5-aminolevulinic acid hydrochloride; Acidum aminolaevulinicum hydrochloricum

Special notes

When selecting the *5-aminolevulinic acid hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-6679-5 *European Pharmacopoeia 9th Edition, Basic Version 2017* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA004 *Erstellung und Validierung eines IdentModul-Updates*
Appendix F [Addition to the second-stage models](#)

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, 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 *5-aminolevulinic acid hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	5-aminolevulinic...	13K27-N02	21339	40	20131125
Caelo	5-aminolevulinic...	16357904	23208	40	1707616
Fagron	5-aminolevulinic...	17A12-B07-332960	23403	40	20170131

Validation samples

A total of 280317 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 *5-aminolevulinic acid hydrochloride*. These samples are listed above in the [calibration samples](#) section.
- 74376 spectra from a total of 1620 batches from further 372 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 *5-aminolevulinic acid hydrochloride*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	5-aminolevulinic acid hydroc...	17A12-B07-332960	23404	40
Caelo	5-aminolevulinic acid hydroc...	16357904	23747	40
Fagron	5-aminolevulinic acid hydroc...	18C16-B05-347714	24099	40

- 126772 spectra from a total of 2786 batches from further 781 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 19 *Apo-Ident* customers from 35 batches from the substance/substance group *5-aminolevulinic acid hydrochloride*.

Supplier	Substance	Batch	Spectra
Fagron	5-aminolevulinic acid hydroc...	12c23-n05	1
Caelo	5-aminolevulinic acid hydroc...	11355616	1
Caelo	5-aminolevulinic acid hydroc...	12093205	2

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Supplier	Substance	Batch	Spectra
Fagron	5-aminolevulinic acid hydroc...	12K26-N05	1
Fagron	5-aminolevulinic acid hydroc...	12H20-N01	1
Fagron	5-aminolevulinic acid hydroc...	13C19-N05	3
Fagron	5-aminolevulinic acid hydroc...	11I30-N01	1
Fagron	5-aminolevulinic acid hydroc...	7447	1
Caelo	5-aminolevulinic acid hydroc...	12093208	1
Fagron	5-aminolevulinic acid hydroc...	13H13-N07	2
Caelo	5-aminolevulinic acid hydroc...	13017402	1
Fagron	5-aminolevulinic acid hydroc...	13J29-N03	2
Fagron	5-aminolevulinic acid hydroc...	13K27-N02	2
Caelo	5-aminolevulinic acid hydroc...	13K27-N02	1
Caelo	5-aminolevulinic acid hydroc...	13017403	1
Caelo	5-aminolevulinic acid hydroc...	14145003	2
Caelo	5-aminolevulinic acid hydroc...	14145007	2
Fagron	5-aminolevulinic acid hydroc...	14K04-B01-297971	2
	5-aminolevulinic acid hydroc...	13C-19-N07	1
Fagron	5-aminolevulinic acid hydroc...	14K13-B01	1
Caelo	5-aminolevulinic acid hydroc...	14145011	1
Fagron	5-aminolevulinic acid hydroc...	15C06-B02-305245	1
Caelo	5-aminolevulinic acid hydroc...	15254803	1
Fagron	5-aminolevulinic acid hydroc...	15J23-B06	1
Fagron	5-aminolevulinic acid hydroc...	16A11-B02-318406	1
Fagron	5-aminolevulinic acid hydroc...	16A11-B02-317459	3
Fagron	5-aminolevulinic acid hydroc...	16I12-B06	1
Fagron	5-aminolevulinic acid hydroc...	16A11-B02-316734	1
Fagron	5-aminolevulinic acid hydroc...	15J23-B06-314284	1
Fagron	5-aminolevulinic acid hydroc...	16G27-B10	1
Fagron	5-aminolevulinic acid hydroc...	17A12-B07-331745	1
Fagron	5-aminolevulinic acid hydroc...	17F01-B06-337164	2
Fagron	5-aminolevulinic acid hydroc...	17F01-B06337165	1
Fagron	5-aminolevulinic acid hydroc...	17F01-B05-338204	1
Fagron	5-aminolevulinic acid hydroc...	17A12-B07-331744	1
Fagron	5-aminolevulinic acid hydroc...	17L18-B05-344673	1

- 78 881 spectra from 565 *Apo-Ident* customers from a total of 26 102 batches from a further 693 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *5-aminolevulinic acid hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *5-aminolevulinic acid hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	74 376
Type B	0	120	0	126 772
Type C	0	45	3	78 881

The substance/substance group *5-aminolevulinic acid hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9887 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9901 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.8817 %)	93.7500 % (> 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
21339	23208	17.17	100.52
23208	23208	0.00	89.39
23403	23208	10.48	88.78

Appendix A: Additional calibration samples (*Type A*)

Substance (spectra also enter the generation of the [chemometric model](#) which cannot be identified with this model. This serves the purpose that substances which the model is not supposed to recognise are safely rejected. The spectra of these samples are entered into the validation as *Type A*. They were recorded by *HiperScan GmbH*.

The samples originate from 157 batches. From these, 6330 spectra were recorded. The calibration spectra of substances which can be identified with the model are listed respectively in the section *calibration samples* for the individual substances and do not appear again elsewhere in this list.

Supplier	Substance	Batch	Spectra	Certificate
Auropure Life...	Amygdalin, bitte...	PA02099-17102131	40	from supplier
Caelo	Amphetamine sulf...	16153902	40	2017A-03361
Caelo	Amphetamine sulf...	13344603	40	0814J-03361
Caelo	Amphetamine sulf...	13344603	40	0814J-03361
Caelo	Bilberry fruit, ...	10265602	40	not necessary
Caelo	Black mustard se...	12350204	80	1403711
Caelo	Cocaine hydrochl...	15224802	40	1316Q-01278
Caelo	Cocaine hydrochl...	15224802	40	1316Q-01278
Caelo	Cocaine hydrochl...	15224802	40	1316Q-01278
Caelo	Cocaine hydrochl...	13259305	40	0814J-01278
Caelo	Cocaine hydrochl...	13259305	40	0814J-01278
Caelo	Cocaine hydrochl...	15224802	40	1316Q-01278
Caelo	Cocaine hydrochl...	17003902	40	1917S-01278
Caelo	Codeine phosphat...	15350703	30	1316R-01279
Caelo	Codeine phosphat...	13071504	40	0814J-01279
Caelo	Codeine phosphat...	15350703	40	1316R-01279
Caelo	Codeine phosphat...	13071504	40	0814J-01279
Caelo	Dihydrocodeine h...	15295901	40	1316Q-03065
Caelo	Dihydrocodeine h...	15295901	40	1316Q-03065
Caelo	Dihydrocodeine h...	13267601	40	0914A-03065
Caelo	Dihydrocodeine h...	12142506	40	0914B-03065
Caelo	Dihydrocodeine h...	12142506	40	0914B-03065
Caelo	Dihydrocodeine h...	13267601	40	0914A-03065
Caelo	Hydromorphone hy...	13267702	40	0914A-01334
Caelo	Hydromorphone hy...	15393602	40	1516J-01334
Caelo	Hydromorphone hy...	13267702	40	0914A-01334
Caelo	Hydromorphone hy...	15393602	40	1516J-01334
Caelo	Ispaghula husk	13238005	40	not necessary
Caelo	Kelp, cut	15418801	60	AR-17-FG-007505-01
Caelo	Kelp, cut	13230805	40	AR-15-FG-007678-01
Caelo	Methadone hydroc...	12344818	40	0914E-02949
Caelo	Methadone hydroc...	15244715	40	1516A-02949
Caelo	Methadone hydroc...	12344818	40	0914E-02949
Caelo	Methadone hydroc...	15244715	40	1516A-02949
Caelo	Midazolam hydroc...	12215811	40	0914E-03538
Caelo	Midazolam hydroc...	12215811	40	0914E-03538
Caelo	Midazolam hydroc...	15224602	40	1516B-03538
Caelo	Midazolam hydroc...	15224602	40	1516B-03538
Caelo	Morphine hydroch...	13349505	40	0914F-01879
Caelo	Morphine hydroch...	16184605	40	1917S-01879
Caelo	Morphine hydroch...	15439404	40	1416R-01879
Caelo	Morphine hydroch...	13349505	40	0914F-01879
Caelo	Morphine hydroch...	15439404	40	1416R-01879
Caelo	Morphine hydroch...	13125207	40	0914E-01879
Caelo	Morphine hydroch...	13125207	40	0914E-01879
Caelo	Morphine sulfate	11333103	40	0914E-07776
Caelo	Morphine sulfate	12153212	40	0914F-07776
Caelo	Morphine sulfate	15255703	40	1416Q-07776

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Morphine sulfate	11333103	40	0914E-07776
Caelo	Morphine sulfate	15255703	40	1416Q-07776
Caelo	Oxycodone hydroc...	12268908	40	0914E-07734
Caelo	Oxycodone hydroc...	12268913	40	1416R-07734
Caelo	Oxycodone hydroc...	12034515	40	0914F-07734
Caelo	Oxycodone hydroc...	12268914	40	1416Q-07734
Caelo	Oxycodone hydroc...	12268914	40	1416Q-07734
Caelo	Oxycodone hydroc...	12268913	40	1416R-07734
Caelo	Oxycodone hydroc...	12268908	40	0914E-07734
Caelo	Oxycodone hydroc...	12034515	40	0914F-07734
Caelo	Phenobarbital	12173202	40	0914E-01040
Caelo	Phenobarbital	12173202	40	0914E-01040
Caelo	Siam benzoin	12321312	40	pending
Caelo	Zinc stearate	180628	40	20180322*
Dr. Behr	L-carnitine hydr...	WE11030091	40	from supplier
Dr. Behr	L-carnitine tart...	WE11060069	40	from supplier
Dr. Behr	L-carnitine tart...	WE15080050	40	from supplier
Euro OTC	Griffonia seed e...	1205027	40	from supplier
Euro OTC	Griffonia seed e...	1705007	40	20170601*
Euro OTC	L-carnitine tart...	1302017-01	40	from supplier
Fagron	Amphetamine sulf...	15L01-B05-315291	40	1316Q-03361
Fagron	Amphetamine sulf...	13G08-N11	40	0814K-03361
Fagron	Amphetamine sulf...	15L01-B05-315291	40	1316Q-03361
Fagron	Amphetamine sulf...	13G08-N11	40	0814K-03361
Fagron	Barbital sodium	12F27-N02	40	0814I-07775
Fagron	Barbital sodium	12F27-N02	40	0814I-07775
Fagron	Barbital sodium	14K14-B04-303353	40	1516I-07775
Fagron	Barbital sodium	14K14-B04-303353	40	1516I-07775
Fagron	Cocaine hydrochl...	13I17-N02	40	0814I-01278
Fagron	Cocaine hydrochl...	13I17-N02	40	0814I-01278
Fagron	Codeine phosphat...	15F09-B02-310520	40	1316Q-01279
Fagron	Codeine phosphat...	15F09-B02-310520	40	1316Q-01279
Fagron	Codeine phosphat...	13C11-N10	40	0814I-01279
Fagron	Codeine phosphat...	13C11-N10	40	0814I-01279
Fagron	Codeine phosphat...	16E17-B05-324109	40	2017A-01279
Fagron	Dexamphetamine s...	15H06-B04-313862	40	1316Q-03582
Fagron	Dexamphetamine s...	13I23-N01	40	0814M-03582
Fagron	Dexamphetamine s...	13I23-N01	40	0814M-03582
Fagron	Dexamphetamine s...	15H06-B04-313862	40	1316Q-03582
Fagron	Dexamphetamine s...	16D20-B01-321049	40	2017B-03582
Fagron	Dihydrocodeine h...	13H19-N03	40	0914C-03065
Fagron	Dihydrocodeine h...	15F18-B07-323388	40	2017A-03065
Fagron	Dihydrocodeine h...	13H19-N03	40	0914C-03065
Fagron	Dihydrocodeine h...	14K26-B04-306298	40	1516I-03065
Fagron	Fentanyl citrate	13G30-N06	40	0814M-07678
Fagron	Fentanyl citrate	15F18-B01-525098	40	1316R-03686
Fagron	Fentanyl citrate	15F18-B01-525166	40	1316Q-03686
Fagron	Fentanyl citrate	15F18-B01-525166	40	1316Q-03686
Fagron	Fentanyl citrate	15F18-B01-525098	40	1316R-03686
Fagron	Fentanyl citrate	13G30-N06	40	0814M-07678
Fagron	Hydromorphone hy...	15L08-B08-316877	40	1917Q-01334
Fagron	Hydromorphone hy...	13I25-N05	40	1516I-01334
Fagron	Hydromorphone hy...	13I25-N05	40	1516I-01334
Fagron	Hydromorphone hy...	13E16-N02	40	0914B-01334
Fagron	Hydromorphone hy...	13E16-N02	40	0914B-01334
Fagron	Methadone hydroc...	15E29-B02-313098	40	1516B-02949
Fagron	Methadone hydroc...	16F24-B02-323183	40	1917Q-02949
Fagron	Methadone hydroc...	13J24-B06	40	0914F-02949
Fagron	Methadone hydroc...	15E29-B02-313098	40	1516B-02949
Fagron	Methadone hydroc...	13J24-B06	40	0914F-02949

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Supplier	Substance	Batch	Spectra	Certificate
Fagron	Midazolam	13K05-N01	40	0914E-07393
Fagron	Midazolam	14C12-B31-313222	40	1516A-07393
Fagron	Midazolam	14C12-B31-313222	40	1516A-07393
Fagron	Midazolam	13K05-N01	40	0914E-07393
Fagron	Midazolam hydroc...	13E22-N09	40	0914F-03538
Fagron	Midazolam hydroc...	14L23-B04-300245	40	1516A-03538
Fagron	Midazolam hydroc...	16C14-B12-332469	40	0718E-03538
Fagron	Midazolam hydroc...	13E22-N09	40	0914F-03538
Fagron	Midazolam hydroc...	14L23-B04-300245	40	1516A-03538
Fagron	Midazolam hydroc...	15H04-B03-314396	40	1917R-03538
Fagron	Midazolam hydroc...	16C14-B12-332469	40	0718E-03538
Fagron	Morphine hydroch...	15I09-B08-312694	40	1416Q-01879
Fagron	Morphine hydroch...	15I09-B08-312694	40	1416Q-01879
Fagron	Morphine hydroch...	13G08-N04	40	0914G-01879
Fagron	Morphine hydroch...	13G08-N04	40	0914G-01879
Fagron	Morphine sulfate	13J07-N04	40	0914G-07776
Fagron	Morphine sulfate	13J07-N04	40	0914G-07776
Fagron	Phenobarbital	15G07-B06-311718	40	1416Q-01040
Fagron	Phenobarbital	15G07-B06-311718	40	1416Q-01040
Flora Apothek...	Amygdalin	13121802	40	1405619
Flora Apothek...	Calcium colamine...	14384	40	from supplier
Flora Apothek...	Glycyrrhizic acid	10588	40	from supplier
Safic-Alcan	Amygdalin, bitte...	BAE150902	40	from supplier
Safic-Alcan	Amygdalin, bitte...	BAE150902	40	from supplier
Safic-Alcan	Dimercaptosuccin...	20170210	40	from supplier
Th. Geyer	Amphetamine sulf...	67002	40	0814I-03361
Th. Geyer	Amphetamine sulf...	67002	40	0814I-03361
Th. Geyer	Calcium colamine...	66606	40	from supplier
Th. Geyer	Calcium colamine...	33299	40	from supplier
Th. Geyer	Cocaine hydrochl...	60145	40	0814K-01278
Th. Geyer	Cocaine hydrochl...	60145	40	0814K-01278
Th. Geyer	Codeine phosphat...	67038	40	0814K-01279
Th. Geyer	Codeine phosphat...	67038	40	0814K-01279
Th. Geyer	Dihydrocodeine h...	67035	40	0914D-03065
Th. Geyer	Dihydrocodeine h...	067052	40	2017D-03065
Th. Geyer	Dihydrocodeine h...	67035	40	0914D-03065
Th. Geyer	Methadone hydroc...	67047	40	0914H-02949
Th. Geyer	Methadone hydroc...	67033	40	0914G-02949
Th. Geyer	Methadone hydroc...	67047	40	0914H-02949
Th. Geyer	Methadone hydroc...	67033	40	0914G-02949
Th. Geyer	Mg-Ca-K colamine...	36985	40	from supplier
Th. Geyer	Mg-Ca-K colamine...	80919	40	from supplier
Th. Geyer	Mg-Ca-K colamine...	46816	40	from supplier
Th. Geyer	Morphine hydroch...	67036	40	0914H-01879
Th. Geyer	Morphine hydroch...	67036	40	0914H-01879
Th. Geyer	Phenobarbital	67045	40	0914F-01040
Th. Geyer	Phenobarbital	067056	40	2017A-01040
Th. Geyer	Phenobarbital	67045	40	0914F-01040
Yino Pharma	Sodium chondroit...	YN010511806006	40	20180912

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Appendix B: Additional validation samples (*Type B*)

It is necessary that spectra also enter the validation which cannot be identified with this model. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded by *HiperScan GmbH*. They are allocated to the *Type B*. They also include the calibration spectra for other models.

The samples originate from 921 batches. From these 38 607 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
abcr GmbH	Amygdalin	1310927	40	from supplier
abcr GmbH	Amygdalin	1310579	40	from supplier
abcr GmbH	Dimercaptosuccin...	1005874	39	from supplier
abcr GmbH	Glycyrrhizic acid	1222024	40	from supplier
AppliChem	Papain	1G000215	40	1407433
Audor	Chlorprothixene ...	AP04120418C	40	not necessary
Audor	Chlorprothixene ...	AP05061117C	40	1810394
Audor	Fluconazole	AP061502911F	40	not necessary
Audor	Fluconazole	AP061502911F	60	AR-16-FG-008733-01
Audor	Fluconazole	APAFLNC0217023F	40	not necessary
Audor	Fluconazole	AP061502911F	40	not necessary
Audor	Fluconazole	AP061502911F	40	not necessary
Audor	Fluconazole	AP061502911F	60	not necessary
Audor	Fluconazole	AP061502911F	40	AR-16-FG-014225-01
Auropure Life...	Amygdalin, bitte...	PA02099-160822	30	from supplier
Bombastus	Bitter fennel	289870	60	AR-15-FG-008161-01
Bombastus	Maize style, cut	274920	40	not necessary
Caelo	Acorus root, nat...	12076404	40	not necessary
Caelo	Acorus root, pee...	12295902	40	not necessary
Caelo	Acorus root, pee...	12239001	40	not necessary
Caelo	Agarikon	14190702	60	not necessary
Caelo	Agarikon	11024502	40	not necessary
Caelo	Agarikon	14190706	60	not necessary
Caelo	Agarikon	13130602	48	1405003
Caelo	Agnus castus fruit	12274003	40	1501649
Caelo	Agnus castus fruit	13193401	40	AR-15-FG-006453-01
Caelo	Agnus castus fruit	15318705	60	pending
Caelo	Agrimony, cut	10325505	45	not necessary
Caelo	Agrimony, cut	11374004	40	not necessary
Caelo	Alchemilla alpin...	12147201	40	not necessary
Caelo	Alchemilla, cut	12153306	40	not necessary
Caelo	Allspice, powder...	12042703	40	not necessary
Caelo	Almonds, bitter,...	13220401	40	1406296
Caelo	Aloes, cape, cut	14087106	60	pending
Caelo	Aloes, cape, cut	11048808	40	pending
Caelo	Aloes, cape, pow...	11132115	40	1404400
Caelo	Aloes, cape, pow...	11132115	40	not necessary
Caelo	Aloes, cape, pow...	12183008	40	not necessary
Caelo	Aluminium oxide,...	12163019	40	not necessary
Caelo	Aluminium oxide,...	13119121	40	not necessary
Caelo	Aluminium potass...	12144605	40	from supplier
Caelo	Ammonium chloride	12356101	40	not necessary
Caelo	Ammonium hydroge...	182108	40	20180926*
Caelo	Amphetamine sulf...	16153902	40	2017A-03361
Caelo	Amphetamine sulf...	13344603	20	0814J-03361
Caelo	Angelica root	12080404	40	1403053
Caelo	Angelica root	12168701	40	pending
Caelo	Angelica root	12080409	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Aniseed	13333903	40	not necessary
Caelo	Aniseed	11370301	40	not necessary
Caelo	Aniseed, pounded	12111301	40	not necessary
Caelo	Aniseed, pounded	13357101	40	not necessary
Caelo	Aniseed, powdered	11306203	40	not necessary
Caelo	Apple, cut	11229807	60	from supplier
Caelo	Arnica flower	11259801	40	not necessary
Caelo	Arnica flower	11285702	40	not necessary
Caelo	Artichoke leaf, ...	13310707	40	not necessary
Caelo	Artichoke leaf, ...	12173302	40	not necessary
Caelo	Ash leaf, cut	11031303	40	not necessary
Caelo	Asparagus root, ...	10299010	40	pending
Caelo	Barberries	11058309	40	pending
Caelo	Barberries	12217109	60	pending
Caelo	Barberries	14057312	60	1508391
Caelo	Barberry root ba...	12112601	40	not necessary
Caelo	Barium sulfate	1711113	40	20170509*
Caelo	Basil, rubbed	12066404	50	not necessary
Caelo	Bean shells, cut	11030601	50	not necessary
Caelo	Bearberry leaf, ...	12186502	40	not necessary
Caelo	Bentonite	12237603	40	not necessary
Caelo	Benzalkonium chl...	16171603	40	not necessary
Caelo	Betony herb, cut	12007205	60	not necessary
Caelo	Betony herb, cut	12007205	40	not necessary
Caelo	Bilberry leaf, cut	12140206	40	not necessary
Caelo	Birch leaf, cut	12193105	40	not necessary
Caelo	Bitter fennel	161603	60	20160718*
Caelo	Bitter fennel	13413702	40	1412549
Caelo	Bitter fennel	12094708	40	pending
Caelo	Bitter fennel	12167102	40	not necessary
Caelo	Bitter fennel	14376403	60	not necessary
Caelo	Bitter fennel	17020610	40	1708048
Caelo	Bitter orange fl...	12266605	40	not necessary
Caelo	Bitter orange fl...	12266703	40	not necessary
Caelo	Bitter orange pe...	12067405	40	not necessary
Caelo	Black cohosh, cut	13237903	40	not necessary
Caelo	Black cohosh, cut	13237901	40	pending
Caelo	Black cohosh, cut	10281112	40	not necessary
Caelo	Black cumin seed	11233503	40	1403495
Caelo	Black cumin seed	161157	60	not necessary
Caelo	Black mustard seed	12189303	40	1403472
Caelo	Black mustard seed	15120405	60	AR-17-FG-007964-01
Caelo	Black mustard se...	13358304	40	pending
Caelo	Black mustard se...	16051807	60	9887
Caelo	Black pepper	11193905	40	not necessary
Caelo	Black pepper	12192311	40	1403490
Caelo	Black pepper	13221114	40	not necessary
Caelo	Blackberry leaf,...	11030707	40	not necessary
Caelo	Blackcurrant lea...	12168804	40	not necessary
Caelo	Blackcurrants	14212502	60	not necessary
Caelo	Blackcurrants	14212509	60	20140829
Caelo	Blackcurrants	12272801	40	1403468
Caelo	Blackthorn flower	12178101	40	not necessary
Caelo	Blessed thistle,...	12038203	40	not necessary
Caelo	Blue bottle flow...	13241902	60	AR-15-FG-005838-01
Caelo	Blue bottle flow...	10291105	40	pending
Caelo	Bogbean leaf, cut	12226101	40	not necessary
Caelo	Boldo leaf, cut	13367904	40	not necessary
Caelo	Borage herb, cut	11206712	40	not necessary
Caelo	Bucho leaf	12034903	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Buprenorphine hy...	16143001	40	2017A-07774
Caelo	Buprenorphine hy...	16143001	40	0718E-07774
Caelo	Buprenorphine hy...	16143001	40	0718E-07774
Caelo	Buprenorphine hy...	12172908	60	0814I-07774
Caelo	Buprenorphine hy...	16143001	40	2017A-07774
Caelo	Buprenorphine hy...	12172908	40	0814I-07774
Caelo	Burdock root, cut	11100801	40	not necessary
Caelo	Burnet root	12027410	40	not necessary
Caelo	Burnet root	12027407	40	not necessary
Caelo	Burnet root	12024406	40	not necessary
Caelo	Calcium chloride...	182411	35	20181022*
Caelo	Calcium hydrogen...	181117	40	20180528*
Caelo	Calcium oxide	182244	39	20181106*
Caelo	Calcium sulfate ...	163363	40	20161214*
Caelo	Calcium sulfate ...	153451	30	20151103*
Caelo	Calendula flower	11221404	40	not necessary
Caelo	Calendula flower...	11187605	40	not necessary
Caelo	Campeche wood	11074105	40	from supplier
Caelo	Caraway fruit	11003217	40	not necessary
Caelo	Caraway fruit	13306006	60	AR-16-FG-000540-03
Caelo	Caraway fruit	13397104	40	AR-15-FG-001526-01
Caelo	Caraway fruit	15097115	60	AR-17-FG-006649-01
Caelo	Caraway fruit	13397104	60	AR-15-FG-001527-01
Caelo	Caraway fruit, p...	14358801	60	AR-15-FG-014914-01
Caelo	Caraway fruit, p...	13367101	40	not necessary
Caelo	Caraway fruit, p...	12116904	40	not necessary
Caelo	Caraway fruit, p...	16073201	60	AR-17-FG-006648-01
Caelo	Carbachol	11150302	31	1401147
Caelo	Cardamom fruit	13260504	40	not necessary
Caelo	Cardamom fruit	11309107	40	not necessary
Caelo	Carnauba wax	183330	40	20190114*
Caelo	Carnauba wax	170903	40	20170512*
Caelo	Castoreum, powde...	12137409	40	1402590
Caelo	Castoreum, powde...	13410403	40	not necessary
Caelo	Castoreum, powde...	13410403	40	not necessary
Caelo	Celery root, cut	10270002	40	not necessary
Caelo	Centaury, cut	11097602	40	not necessary
Caelo	Chickweed, cut	13254411	40	1412550
Caelo	Chickweed, cut	13040502	40	1403482
Caelo	Chicory herb, cut	12034303	60	not necessary
Caelo	Chicory herb, cut	12354302	100	not necessary
Caelo	Chicory root, cut	11374504	40	not necessary
Caelo	Cinchona bark, cut	15301903	60	AR-17-FG-007831-01
Caelo	Cinchona bark, cut	13031007	40	not necessary
Caelo	Cinchona bark, cut	14009304	40	AR-15-FG-007677-01
Caelo	Cinchona bark, cut	11238512	40	1403463
Caelo	Cinnamon rods (C...	13241807	40	not necessary
Caelo	Cinnamon, cut	14175010	60	1505349
Caelo	Cinnamon, cut	12309902	40	pending
Caelo	Cinnamon, cut	16114401	60	1704441
Caelo	Cinnamon, cut	13304414	40	not necessary
Caelo	Clove	16207804	60	1708676
Caelo	Clove	12095805	40	pending
Caelo	Cocaine hydrochl...	16142710	40	1917T-01278
Caelo	Cocaine hydrochl...	17003902	40	1917S-01278
Caelo	Cocaine hydrochl...	16142710	40	1917T-01278
Caelo	Cocaine hydrochl...	15224802	20	1316Q-01278
Caelo	Cocaine hydrochl...	15224802	20	1316Q-01278
Caelo	Cocaine hydrochl...	15224802	20	1316Q-01278
Caelo	Cocaine hydrochl...	15224802	20	1316Q-01278

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Cocaine hydrochl...	13259305	20	0814J-01278
Caelo	Codeine phosphat...	16169807	40	2017B-01279
Caelo	Codeine phosphat...	16349702	40	2017C-01279
Caelo	Codeine phosphat...	15350703	20	1316R-01279
Caelo	Codeine phosphat...	16349702	40	2017C-01279
Caelo	Codeine phosphat...	13071504	20	0814J-01279
Caelo	Codeine phosphat...	15350703	30	1316R-01279
Caelo	Codeine phosphat...	16169807	40	2017B-01279
Caelo	Common wormwood ...	12016705	40	not necessary
Caelo	Copper (II) sulf...	162409	40	20160825*
Caelo	Coriander	13299403	40	1412548
Caelo	Coriander	16010212	60	AR-17-FG-015965-01
Caelo	Coriander	12080904	40	pending
Caelo	Cottonwood bud	12027505	40	not necessary
Caelo	Couch grass rhiz...	12186702	40	not necessary
Caelo	Cowberry leaf, cut	11334302	40	not necessary
Caelo	Cumin	11378308	30	not necessary
Caelo	Daisy flower	11068306	40	not necessary
Caelo	Damiana leaf, cut	11026608	40	not necessary
Caelo	Dandelion herb w...	11217109	40	not necessary
Caelo	Dandelion root, ...	13329701	40	not necessary
Caelo	Dandelion root, ...	13329708	40	1411089
Caelo	Dandelion root, ...	12363102	40	1403708
Caelo	Devil's claw root	12031806	40	not necessary
Caelo	Devil's claw root	13298202	40	not necessary
Caelo	Dihydrocodeine h...	15295901	20	1316Q-03065
Caelo	Dihydrocodeine h...	12142506	20	0914B-03065
Caelo	Dihydrocodeine h...	16106209	40	2017C-03065
Caelo	Dihydrocodeine h...	13267601	20	0914A-03065
Caelo	Dihydrocodeine h...	15295910	40	2017B-03065
Caelo	Dihydrocodeine h...	15295910	40	2017B-03065
Caelo	Dihydrocodeine h...	15295901	20	1316Q-03065
Caelo	Dihydrocodeine h...	16106209	40	2017C-03065
Caelo	Dill fruit	12342906	40	not necessary
Caelo	Dill fruit	14018705	60	pending
Caelo	Dill fruit	12289901	40	1403464
Caelo	Dill herb, cut	13007610	40	not necessary
Caelo	Dill herb, cut	11295103	40	not necessary
Caelo	Dill herb, cut	11295107	40	pending
Caelo	Dill herb, cut	13007602	40	1402204
Caelo	Dry beads Caelo...	12382203	40	from supplier
Caelo	Dry beads Caelo...	11005804	40	from supplier
Caelo	Echinacea pallid...	14120602	40	not necessary
Caelo	Echinacea pallid...	12244501	40	not necessary
Caelo	Elder berries	12267807	40	1403466
Caelo	Elder berries	13367704	40	1410179
Caelo	Elder flower, ru...	12221902	40	not necessary
Caelo	Elecampane rhizo...	12113303	40	not necessary
Caelo	Eleutherococcus, ...	10381814	30	not necessary
Caelo	Elm bark, cut	10347205	60	not necessary
Caelo	Emser salt, arti...	181633	40	20180621*
Caelo	Equisetum stem, ...	10375515	40	not necessary
Caelo	Eucalyptus leaf, ...	11307706	40	not necessary
Caelo	Fenugreek	11313204	40	not necessary
Caelo	Fenugreek, powde...	15308704	60	AR-17-FG-006625-01
Caelo	Fenugreek, powde...	12149605	40	not necessary
Caelo	Flax weed herb, ...	13007505	40	1403462
Caelo	Flax weed herb, ...	14005309	60	not necessary
Caelo	Frangula bark, cut	12185901	40	not necessary
Caelo	Frankincense	12120005	40	1402495

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Frankincense	13112801	40	not necessary
Caelo	Fraxinella root,...	10189103	40	not necessary
Caelo	Fraxinella root,...	14110802	60	not necessary
Caelo	Fraxinella root,...	11314705	80	not necessary
Caelo	Fraxinella root,...	11314705	40	pending
Caelo	Fumitory, cut	12103402	40	not necessary
Caelo	Galangal root	11375904	40	not necessary
Caelo	Galangal root	14159504	60	1511617
Caelo	Galangal root	12125001	40	not necessary
Caelo	Galangal root	12330308	40	not necessary
Caelo	Galangal root	11375909	40	1403324
Caelo	Galangal root	12330305	40	1403491
Caelo	Garden violet, cut	10292002	40	pending
Caelo	Garden violet, cut	13038703	40	1403481
Caelo	Garden violet, cut	13232103	40	not necessary
Caelo	Gentian root, cut	12244603	40	not necessary
Caelo	Gentian root, po...	12007106	40	not necessary
Caelo	Gentian root, po...	12007103	50	1403630
Caelo	Gentian root, po...	13410503	40	1508394
Caelo	Ginger, peeled	13321904	40	not necessary
Caelo	Ginger, peeled	14120701	40	not necessary
Caelo	Ginger, peeled	12180601	40	not necessary
Caelo	Ginger, peeled	11325715	40	not necessary
Caelo	Ginkgo extract	12192505	40	1403672
Caelo	Ginkgo leaf, cut	13340907	60	not necessary
Caelo	Ginkgo leaf, cut	16281501	60	1708047
Caelo	Ginkgo leaf, cut	12151703	40	not necessary
Caelo	Ginkgo leaf, cut	13340904	40	1411088
Caelo	Ginseng root	11349206	40	not necessary
Caelo	Ginseng root	12080208	40	not necessary
Caelo	Ginseng root	13341008	40	not necessary
Caelo	Ginseng root	13237805	40	not necessary
Caelo	Guaiacum wood, cut	13343802	40	not necessary
Caelo	Guaiacum wood, cut	11352012	40	not necessary
Caelo	Guaiacum wood, cut	11352001	40	1406340
Caelo	Hamamelis bark, ...	12361303	40	not necessary
Caelo	Hamamelis bark, ...	12361301	40	not necessary
Caelo	Hamamelis leaf, ...	10102915	40	not necessary
Caelo	Hamamelis leaf, ...	13269904	40	not necessary
Caelo	Hamamelis leaf, ...	13269902	40	1405176
Caelo	Hawthorn flower	10157201	40	not necessary
Caelo	Hawthorn flower	13010403	40	not necessary
Caelo	Hawthorn fruit	11278205	30	not necessary
Caelo	Hawthorn fruit	11183010	40	not necessary
Caelo	Hawthorn leaf wi...	10273515	40	not necessary
Caelo	Hawthorn leaf wi...	10273513	40	not necessary
Caelo	Hawthorn leaf wi...	13276706	40	not necessary
Caelo	Hay flower	12317104	40	not necessary
Caelo	Heather flower, ...	10270508	40	not necessary
Caelo	Heather, cut	11011209	40	not necessary
Caelo	Heavy alkaline b...	181942	40	20181010*
Caelo	Henna powder	12267304	40	from supplier
Caelo	Henna powder	12122302	40	from supplier
Caelo	Hop strobile	12221802	40	not necessary
Caelo	Hop strobile	12008305	40	not necessary
Caelo	Horse chestnut l...	11063503	40	not necessary
Caelo	Hydromorphone hy...	15393602	20	1516J-01334
Caelo	Hydromorphone hy...	15393602	20	1516J-01334
Caelo	Hydromorphone hy...	13267702	20	0914A-01334
Caelo	Hydromorphone hy...	16123804	40	1917R-01334

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Hydromorphone hy...	16123804	40	1917R-01334
Caelo	Hydroxyethylcell...	181131	40	20180612*
Caelo	Hydroxyethylcell...	17115103	40	not necessary
Caelo	Hydroxyethylcell...	171151	40	20170523*
Caelo	Iceland moss, cut	13350803	40	not necessary
Caelo	Iceland moss, cut	12187106	40	1403493
Caelo	Iodine	181635	40	20180704*
Caelo	Iron (II) sulfat...	11340509	40	1401568
Caelo	Iron (III) chlor...	12354703	40	1401391
Caelo	Iron (III) sulfa...	170991	40	20170523*
Caelo	Isomalt	170812	40	20170421*
Caelo	Ispaghula husk	12148103	40	not necessary
Caelo	Ispaghula seed	11185807	40	not necessary
Caelo	Ivy leaf, cut	11229505	40	not necessary
Caelo	Ivy leaf, cut	13276304	40	not necessary
Caelo	Jasmine flower	12143201	40	not necessary
Caelo	Java tea, cut	13258805	40	not necessary
Caelo	Java tea, cut	12225702	40	not necessary
Caelo	Juniper	13267210	40	not necessary
Caelo	Juniper	12028609	40	not necessary
Caelo	Juniper, pounded	12278903	40	1405296
Caelo	Juniper, pounded	13367302	40	not necessary
Caelo	Kaolin, heavy	11350124	40	not necessary
Caelo	Kaolin, red, pow...	12093503	40	from supplier
Caelo	Kidney vetch, co...	10249206	40	not necessary
Caelo	Knotgrass, cut	14079304	40	not necessary
Caelo	Ladys bedstraw ...	11265103	40	not necessary
Caelo	Lapacho wood, cut	12239305	40	not necessary
Caelo	Lapis Pumicis	180533	40	20180222*
Caelo	Laurel leaf	12299103	40	not necessary
Caelo	Lavender flower	12088003	60	not necessary
Caelo	Lavender flower	13336005	40	from supplier
Caelo	Lemon peel, cut	12217402	40	not necessary
Caelo	Lemon verbena le...	12137505	40	not necessary
Caelo	Lemon verbena le...	12137503	40	not necessary
Caelo	Lime flower, cut	11086305	55	not necessary
Caelo	Linseed	12186902	60	pending
Caelo	Linseed	13296703	40	not necessary
Caelo	Linseed	12092102	60	not necessary
Caelo	Linseed	13412801	40	not necessary
Caelo	Liquorice root, ...	12227101	40	not necessary
Caelo	Liquorice root, ...	11351911	40	not necessary
Caelo	Liquorice root, ...	12227106	40	not necessary
Caelo	Liquorice	13180904	60	pending
Caelo	Liquorice	14050601	60	not necessary
Caelo	Liquorice	13068904	40	not necessary
Caelo	Liquorice root, ...	12267103	40	not necessary
Caelo	Locust bean gum,...	13379403	40	from supplier
Caelo	Locust bean gum,...	10376516	40	not necessary
Caelo	Lovage root, cut	11181609	40	not necessary
Caelo	Magensium hydrog...	12181911	40	not necessary
Caelo	Magnesium carbon...	182282	40	20180906*
Caelo	Magnesium hydrox...	16253301	30	not necessary
Caelo	Magnesium oxide,...	180818	40	20180322*
Caelo	Magnesium sulfat...	13340814	60	not necessary
Caelo	Magnesium sulfat...	172990	40	20171129*
Caelo	Maize style, cut	13381501	40	not necessary
Caelo	Maize style, cut	10325906	40	not necessary
Caelo	Male speedwell w...	12162503	40	not necessary
Caelo	Mallow flower, cut	12187405	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Mallow leaf, cut	12153403	40	not necessary
Caelo	Manganese sulfat...	171648	40	20170714*
Caelo	Manna, cut	13127007	40	pending
Caelo	Manna, cut	11308907	60	pending
Caelo	Manna, powdered	14001401	40	not necessary
Caelo	Manna, powdered	11308807	40	1403534
Caelo	Marian thistle f...	11126703	40	not necessary
Caelo	Marian thistle f...	13342002	40	from supplier
Caelo	Marian thistle h...	10365601	40	not necessary
Caelo	Marshmallow leaf...	12328206	40	not necessary
Caelo	Marshmallow root...	13214804	40	not necessary
Caelo	Marshmallow root...	11101905	40	not necessary
Caelo	Masterwort root,...	12101804	60	not necessary
Caelo	Masterwort root,...	13341204	40	not necessary
Caelo	Maté leaf, cut	13118004	40	not necessary
Caelo	Maté leaf, cut	11091707	40	not necessary
Caelo	Matricaria flower	12294804	40	not necessary
Caelo	Matricaria flower	12337605	40	not necessary
Caelo	Matricaria flowe...	12115805	40	not necessary
Caelo	Meadowsweet flow...	12275701	40	not necessary
Caelo	Medical coal	181885	40	20180813*
Caelo	Melissa leaf, cut	13214713	40	not necessary
Caelo	Melissa leaf, cut	12032318	40	not necessary
Caelo	Methadone hydroc...	16135309	40	1917R-02949
Caelo	Methadone hydroc...	12344818	20	0914E-02949
Caelo	Methadone hydroc...	15244715	20	1516A-02949
Caelo	Methadone hydroc...	15244715	20	1516A-02949
Caelo	Methadone hydroc...	16135309	40	1917R-02949
Caelo	Methylrosanilini...	12276308	40	1509299
Caelo	Midazolam hydroc...	12215811	20	0914E-03538
Caelo	Midazolam hydroc...	15224602	20	1516B-03538
Caelo	Midazolam hydroc...	15224602	20	1516B-03538
Caelo	Midazolam hydroc...	15224611	40	1917S-03538
Caelo	Midazolam hydroc...	15224611	30	1917S-03538
Caelo	Mistletoe, cut	11294003	30	not necessary
Caelo	Morphine hydroch...	15439404	20	1416R-01879
Caelo	Morphine hydroch...	15439404	20	1416R-01879
Caelo	Morphine hydroch...	15439411	40	1917R-01879
Caelo	Morphine hydroch...	15439411	40	1917R-01879
Caelo	Morphine hydroch...	13349505	20	0914F-01879
Caelo	Morphine hydroch...	13125207	20	0914E-01879
Caelo	Morphine hydroch...	16184605	40	1917S-01879
Caelo	Morphine sulfate	15295802	40	1917R-07776
Caelo	Morphine sulfate	15295802	40	1917R-07776
Caelo	Morphine sulfate	11333103	20	0914E-07776
Caelo	Morphine sulfate	15255703	20	1416Q-07776
Caelo	Morphine sulfate	12153212	60	0914F-07776
Caelo	Morphine sulfate	15255703	20	1416Q-07776
Caelo	Mullein flower	11366403	40	not necessary
Caelo	Mullein flower, ...	11233402	60	not necessary
Caelo	Myrrh	11277111	60	1403081
Caelo	Myrrh	13108701	40	AR-15-FG-000946-01
Caelo	Myrrh	12269901	40	1403470
Caelo	Nettle leaf, cut	12184702	40	not necessary
Caelo	Nettle root, cut	11254903	40	not necessary
Caelo	Nettle seed	11126211	40	pending
Caelo	Nettle seed	12131507	40	1402203
Caelo	Nettle seed	13387110	40	1410300
Caelo	Nutmeg	12067304	40	not necessary
Caelo	Nutmeg	13266002	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Oak bark, cut	10348617	40	not necessary
Caelo	Oak bark, cut	13360306	40	not necessary
Caelo	Oak bark, cut	11351207	40	1403492
Caelo	Oak bark, powdered	11235004	40	not necessary
Caelo	Oat straw, cut	11280008	40	not necessary
Caelo	Olive leaf	12316808	60	AR-15-FG-001051-01
Caelo	Olive leaf	11270106	40	not necessary
Caelo	Orris root	12206802	40	not necessary
Caelo	Orris root	11026705	40	not necessary
Caelo	Oxycodone hydroc...	15220205	40	2017A-07734
Caelo	Oxycodone hydroc...	12268913	20	1416R-07734
Caelo	Oxycodone hydroc...	12268914	20	1416Q-07734
Caelo	Oxycodone hydroc...	12268914	20	1416Q-07734
Caelo	Oxycodone hydroc...	12034515	20	0914F-07734
Caelo	Oxycodone hydroc...	12268913	20	1416R-07734
Caelo	Oxycodone hydroc...	12268908	20	0914E-07734
Caelo	Oxycodone hydroc...	15220205	40	2017A-07734
Caelo	Parsley root, cut	12080301	40	not necessary
Caelo	Peppermint leaf,...	12321503	130	not necessary
Caelo	Peppermint leaf,...	11347607	40	not necessary
Caelo	Peppermint leaf,...	11294401	40	not necessary
Caelo	Peppermint leaf,...	13288303	40	not necessary
Caelo	Phenobarbital	12173202	20	0914E-01040
Caelo	Pine sprouts, cut	13256105	40	not necessary
Caelo	Pine sprouts, cut	11164708	60	not necessary
Caelo	Piper cubeba	11081903	40	not necessary
Caelo	Podophyllum resi...	12287810	40	1405242
Caelo	Potassium bromide	11208211	40	not necessary
Caelo	Potassium carbon...	180995	40	20180412*
Caelo	Potassium hydrog...	172493	40	20170911*
Caelo	Potassium hydrox...	180083	40	20180118*
Caelo	Potassium iodide	11090222	40	not necessary
Caelo	Potassium metabi...	12325906	40	not necessary
Caelo	Potassium monohy...	12366501	40	10401307
Caelo	Potassium nitrate	12236703	40	not necessary
Caelo	Primrose flower	11268002	40	not necessary
Caelo	Primrose flower	11206806	100	not necessary
Caelo	Primrose root, cut	12064506	40	not necessary
Caelo	Propolis extract...	11124120	40	1403460
Caelo	Propolis extract...	13396103	40	not necessary
Caelo	Propolis extract...	13396103	40	not necessary
Caelo	Psyllium seed	10291205	80	not necessary
Caelo	Psyllium seed	10291206	40	pending
Caelo	Psyllium seed	13305903	40	pending
Caelo	Pumpkin seed, pe...	12249002	40	1404542
Caelo	Pumpkin seed, pe...	12249006	40	not necessary
Caelo	Ramsons herb, cut	12380801	40	1404538
Caelo	Ramsons herb, cut	13072801	40	not necessary
Caelo	Raspberry leaf, ...	12362701	40	not necessary
Caelo	Red poppy petals...	12008104	40	not necessary
Caelo	Red-rose petal	11299204	40	not necessary
Caelo	Red-rose petal, ...	11304912	40	not necessary
Caelo	Redwood	12049604	40	not necessary
Caelo	Restharrow root,...	12330001	40	not necessary
Caelo	Rhubarb, cut	12211906	40	not necessary
Caelo	Rhubarb, cut	13235213	40	not necessary
Caelo	Rhubarb, cut	11057818	40	not necessary
Caelo	Rhubarb, powdered	11043818	60	1403280
Caelo	Rhubarb, powdered	16009901	60	9886
Caelo	Ribwort plantain...	12362902	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Rifampicin	152446	40	20150831*
Caelo	Rifaximin	161053	60	20160607*
Caelo	Rose hips peel, ...	11301407	60	not necessary
Caelo	Rose hips with p...	11232204	40	not necessary
Caelo	Rose hips with p...	12064202	40	not necessary
Caelo	Rose mallow flow...	10244508	60	not necessary
Caelo	Roselle	12007311	60	not necessary
Caelo	Roselle	11036509	60	not necessary
Caelo	Rosemary leaf, cut	14159601	60	not necessary
Caelo	Rosemary leaf, cut	11193408	40	not necessary
Caelo	Sage leaf, cut	11347503	40	not necessary
Caelo	Sarsaparilla roo...	10230402	60	not necessary
Caelo	Senna leaf, cut	12273106	40	not necessary
Caelo	Senna leaf, powd...	11193307	120	pending
Caelo	Senna leaf, powd...	12369908	40	1408079
Caelo	Senna pods, tinn...	13395106	40	not necessary
Caelo	Senna pods, tinn...	11154404	40	not necessary
Caelo	Senna pods, tinn...	12267605	40	not necessary
Caelo	Shepherd's purse...	11328208	40	not necessary
Caelo	Siam benzoin	12321314	40	not necessary
Caelo	Silica, colloida...	181124	40	20180424*
Caelo	Silver nitrate	181276	40	20180716*
Caelo	Silver, colloida...	173615	40	20180312*
Caelo	Silverweed, cut	11328105	40	not necessary
Caelo	Sodium bromide	171191	40	20170510*
Caelo	Sodium carbonate...	173613	40	20180115*
Caelo	Sodium carbonate...	16310205	40	not necessary
Caelo	Sodium dihydroge...	12198506	40	not necessary
Caelo	Sodium iodide	161701	40	20160706*
Caelo	Sodium monohydro...	12109002	40	not necessary
Caelo	Sodium nitrate	11045910	40	not necessary
Caelo	Sodium nitrite	171360	30	20170522*
Caelo	Sodium perborate...	11158903	40	not necessary
Caelo	Sodium thiosulfa...	181648	40	20180712*
Caelo	Solanum dulcamar...	10375602	40	not necessary
Caelo	Solanum dulcamar...	13254305	40	not necessary
Caelo	Sour cherry stem...	12042302	40	1503570
Caelo	Spearmint leaf, ...	12133906	40	not necessary
Caelo	Star anise	11314104	40	not necessary
Caelo	Star anise, cut	12226301	60	pending
Caelo	Star anise, cut	15329302	60	AR-16-FG-004770-01
Caelo	Star anise, cut	13041401	40	1403709
Caelo	Stemless carline...	12163702	40	not necessary
Caelo	Stemless carline...	12232802	40	not necessary
Caelo	Strawberry leaf...	11117903	40	not necessary
Caelo	Sulfamerazine	10218403	30	not necessary
Caelo	Sweet woodruff h...	10375812	30	not necessary
Caelo	Talcum	11318312	80	1405338
Caelo	Theriac, powdered	13407301	40	1410336
Caelo	Theriac, powdered	12289307	40	1405122
Caelo	Thiomersal	172173	30	20170919*
Caelo	Thyme, rubbed	11345004	60	not necessary
Caelo	Tonka beans	12145101	40	not necessary
Caelo	Tormentil	14360103	60	1606520
Caelo	Tormentil	13220502	40	1403049
Caelo	Tormentil	12040708	40	1403487
Caelo	Tormentil	12013103	40	1403048
Caelo	Tormentil	12040715	40	1403710
Caelo	Tragacanth, powd...	13277804	60	1507149
Caelo	Tragacanth, powd...	15085602	60	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Tragacanth, powd...	16110802	60	AR-17-FG-007533-01
Caelo	Tragacanth, powd...	15379906	60	not necessary
Caelo	Tribromophenol b...	18144202	40	not necessary
Caelo	Turmeric root, cut	11160403	60	not necessary
Caelo	Turmeric root, cut	13360202	40	1411363
Caelo	Turmeric root, cut	12136503	40	1405295
Caelo	Turmeric, javane...	12185605	40	1403465
Caelo	Turmeric, javane...	12319206	40	not necessary
Caelo	Turmeric, javane...	13262904	40	not necessary
Caelo	Valerian root, cut	12033809	40	not necessary
Caelo	Valerian root, p...	12138005	40	1403809
Caelo	Valerian root, p...	12138008	40	1508496
Caelo	Valerian root, p...	13113204	60	pending
Caelo	Verbena herb, cut	12187602	40	not necessary
Caelo	Walnut bark, cut	11325603	40	not necessary
Caelo	Walnut leaf, cut	11103007	40	1403091
Caelo	White deadnettle...	11371604	40	not necessary
Caelo	White mustard seed	12361002	40	1403473
Caelo	White mustard seed	13064301	40	pending
Caelo	White mustard seed	13380501	40	not necessary
Caelo	White mustard se...	12375705	40	not necessary
Caelo	White mustard se...	12349601	60	1403281
Caelo	White pepper	12294902	40	1403488
Caelo	White pepper	14010703	40	not necessary
Caelo	White pepper	12294905	40	not necessary
Caelo	Wild pansy, cut	10291007	60	not necessary
Caelo	Willow bark, cut	12185204	40	not necessary
Caelo	Willow herb, cut	11347311	40	not necessary
Caelo	Willowherb, smal...	10326106	40	not necessary
Caelo	Willowherb, smal...	13355904	60	not necessary
Caelo	Wormwood herb, cut	12355801	40	not necessary
Caelo	Yarrow flower, r...	12267703	40	not necessary
Caelo	Yellow chaste we...	11293101	40	not necessary
Caelo	Zedoary root, cut	12125301	40	not necessary
Caelo	Zedoary root, po...	13165501	40	pending
Caelo	Zedoary root, po...	14249001	60	not necessary
Caelo	Zedoary root, po...	12344601	40	1403489
Caelo	Zinc chloride	11345504	40	not necessary
Caelo	Zinc oxide	14038101	40	not necessary
Caelo	Zinc oxide-talcu...	181487	40	20180702*
Caelo	Zinc sulfate hep...	12257802	40	not necessary
Carotech	Tocomax 15%	100912	40	from supplier
Dr. Behr	L-carnitine hydr...	WE11030091	20	from supplier
Dr. Behr	L-carnitine tart...	WE15080050	20	from supplier
Dr. Behr	Quercetin	WE-13030084-02	40	not necessary
Dr. Behr	Yam root extract	WE14020005-05	40	pending
Euro OTC	Ammonium chloride	1209013-01	40	not necessary
Euro OTC	Calcium carbonat...	1611008-01	40	not necessary
Euro OTC	Chromium yeast 0...	L1303028-01	40	1403474
Euro OTC	Chromium yeast 0...	L1406030-02	60	not necessary
Euro OTC	Curcuma extract ...	L1408013	60	not necessary
Euro OTC	Cysteine hydroch...	1304019-01	40	not necessary
Euro OTC	Cysteine hydroch...	1706023	40	20170721*
Euro OTC	Cysteine hydroch...	1510015	60	20151112*
Euro OTC	Cysteine hydroch...	1507006	60	20150713*
Euro OTC	Cysteine hydroch...	1603018	40	20160419*
Euro OTC	Cysteine hydroch...	1701012	40	20170207*
Euro OTC	Cysteine hydroch...	1807010-01	40	not necessary
Euro OTC	D-(+)-mannose	L1111005-02	40	1405612
Euro OTC	D-(+)-mannose	L1111005-02	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Euro OTC	D-(+)-mannose	L1503016-01	60	not necessary
Euro OTC	Deoxycholic acid	1305051-01	40	not necessary
Euro OTC	Devil's claw roo...	1210003-02	40	not necessary
Euro OTC	Devil's claw roo...	1210003-02	40	1707472
Euro OTC	Devil's claw roo...	1210003-02	40	not necessary
Euro OTC	EDTA calcium dis...	1705029	40	20170626*
Euro OTC	EDTA calcium dis...	1807024	40	20180725*
Euro OTC	Frankincense ext...	1602008	60	20160215*
Euro OTC	Frankincense ext...	1611023-01	60	9889
Euro OTC	Frankincense ext...	1308020-01	60	8958
Euro OTC	Frankincense ext...	1602008	60	20160215*
Euro OTC	Griffonia seed e...	1810009	40	20181025*
Euro OTC	Heavy magnesium ...	1709011-02	40	not necessary
Euro OTC	Iron (II) glucon...	1805025	40	20180604*
Euro OTC	L-alanine	1601033-01	40	not necessary
Euro OTC	L-alanine	1710009	40	20171018*
Euro OTC	L-carnitine tart...	1708023	40	20170907*
Euro OTC	Magnesium carbon...	1711011-01	40	not necessary
Euro OTC	Magnesium chlori...	1802023-01	40	not necessary
Euro OTC	Magnesium trisil...	1608024-01	40	not necessary
Euro OTC	Potassium hydroc...	1805027-01	40	not necessary
Euro OTC	Potassium orotate	1203038V-02	60	not necessary
Euro OTC	Potassium orotate	1203038V-02	40	not necessary
Euro OTC	Potassium orotate	1203038V-02	40	9757
Euro OTC	Potassium perman...	1708016-02	40	not necessary
Euro OTC	Ropivacaine hydr...	1707006	40	20171013*
Euro OTC	Selenium disulfide	1411011-02	40	not necessary
Euro OTC	Sodium dihydroge...	1202015-01	40	not necessary
Euro OTC	Sodium hydrogen ...	1807021-01	40	not necessary
Euro OTC	Sodium molybdate...	L1305049-01	45	not necessary
Euro OTC	Sodium molybdate...	L1305049-01	60	not necessary
Euro OTC	Sodium sulfate d...	1708012-02	40	not necessary
Euro OTC	Sodium sulfate, ...	1801046-01	40	not necessary
Euro OTC	Titanium dioxide	1708015-01	40	not necessary
Euro OTC	Tricalcium phosp...	1206002-01	40	1402298
Euro OTC	Zinc orotate dihydro...	1203014-01	40	1407431
Euro OTC	Zinc orotate dihydro...	1203014-01	40	not necessary
Euro OTC	Zinc orotate dihydro...	13050005-02	40	not necessary
Fagron	(R,S)-epinephrin...	14A22-B05-291560	60	no certificate available
Fagron	(R,S)-epinephrin...	16H23-B98-325052	40	not necessary
Fagron	(R,S)-epinephrin...	12H08-N03	40	no certificate available
Fagron	5-fluorouracil	16D01-U05/3-327376	40	not necessary
Fagron	5-fluorouracil	13F19-N03	40	1402308
Fagron	5-fluorouracil	13F19-N03	60	1608169
Fagron	8-quinolinol sul...	12H21-N08	40	not necessary
Fagron	Aluminium chlori...	12I27-N01	40	not necessary
Fagron	Amphetamine sulf...	16A29-B03-324577	40	2017B-03361
Fagron	Amphetamine sulf...	13G08-N11	20	0814K-03361
Fagron	Amphetamine sulf...	16A29-B03-324577	40	2017B-03361
Fagron	Amphetamine sulf...	15L01-B05-315291	20	1316Q-03361
Fagron	Amphetamine sulf...	15L01-B05-315291	20	1316Q-03361
Fagron	Barbital sodium	12F27-N02	20	0814I-07775
Fagron	Barbital sodium	15L07-B02-324539	40	2017A-07775
Fagron	Barbital sodium	14K14-B04-303353	20	1516I-07775
Fagron	Barbital sodium	15L07-B02-324539	40	2017A-07775
Fagron	Barbital sodium	14K14-B04-303353	20	1516I-07775
Fagron	Betaine hydrochl...	13H13-N02	40	1402684
Fagron	Betamethasone-17...	17F12-B10-34942	40	not necessary
Fagron	Bromelain	14F20-B03295501	40	pending
Fagron	Bromelain	14F20-B03295501	60	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Fagron	Bupivacaine hydr...	17E22-B08-345817	40	20170615
Fagron	Caffeine citrate	15A05-B03-318006	40	not necessary
Fagron	Caffeine citrate	15A05-B03-302746	60	not necessary
Fagron	Caffeine citrate	15A05-B03-302746	40	not necessary
Fagron	Caffeine citrate	12C16-N03	40	1403477
Fagron	Caffeine citrate	15A05-B03-318006	40	not necessary
Fagron	Calcium hydroxide	13E22-N07	20	not necessary
Fagron	Chlorhexidine di...	16C11-B02-322510	40	not necessary
Fagron	Chlorhexidine di...	16C11-B02-324203	40	not necessary
Fagron	Chlorhexidine di...	16C11-B02-329881	40	not necessary
Fagron	Chlorhexidine di...	14A09-B03-290724	40	AR-15-FG-012308-01
Fagron	Chlorobutanol he...	14A06-B31-290310	60	1412458
Fagron	Cinchocaine hydr...	13G24-N05	40	not necessary
Fagron	Cinchocaine hydr...	12F25-N10	40	1401148
Fagron	Cinnarizine	14D09-B01-294702	60	AR-16-FG-008930-01
Fagron	Cinnarizine	13H01-N07	40	1402306
Fagron	Cinnarizine	11L22-N13	40	not necessary
Fagron	Clobetasol-17-pr...	13E16-N01	40	not necessary
Fagron	Cocaine hydrochl...	13I17-N02	20	0814I-01278
Fagron	Cocaine hydrochl...	14H27-B03-304551	40	1917R-01278
Fagron	Cocaine hydrochl...	16B11-B05-323386	40	1917Q-1278
Fagron	Cocaine hydrochl...	16B11-B05-323386	40	1917Q-1278
Fagron	Cocaine hydrochl...	14H27-B03-304551	40	1917R-01278
Fagron	Codeine monohydr...	12C05-N05	40	0814I-01280
Fagron	Codeine monohydr...	12C05-N05	60	0814I-01280
Fagron	Codeine phosphat...	13C11-N10	20	0814I-01279
Fagron	Codeine phosphat...	16E17-B05-324109	40	2017A-01279
Fagron	Codeine phosphat...	15F09-B02-310520	20	1316Q-01279
Fagron	Codeine phosphat...	15F09-B02-310520	20	1316Q-01279
Fagron	Cyproheptadine h...	16K07-B01-350645	40	20161202
Fagron	Deoxycholic acid	14A02-B32-303429	60	AR-16-FG-004648-01
Fagron	Deoxycholic acid	14A02-B32-303429	40	not necessary
Fagron	Dexamethasone 1:...	18C13-B06-348239	40	not necessary
Fagron	Dexamphetamine s...	16F09-B02-328352	40	2017A-03582
Fagron	Dexamphetamine s...	15H06-B04-313862	20	1316Q-03582
Fagron	Dexamphetamine s...	13I23-N01	20	0814M-03582
Fagron	Dexamphetamine s...	15H06-B04-313862	20	1316Q-03582
Fagron	Dexamphetamine s...	16F09-B02-328352	40	2017A-03582
Fagron	Dexamphetamine s...	16D20-B01-321049	40	2017B-03582
Fagron	Dihydrocodeine h...	14K26-B04-306298	60	1516I-03065
Fagron	Dihydrocodeine h...	14K26-B04-306298	20	1516I-03065
Fagron	Dihydrocodeine h...	15F18-B07-323388	40	2017A-03065
Fagron	Dihydrocodeine h...	13H19-N03	20	0914C-03065
Fagron	Econazole nitrate	12I06-B40-306925	40	not necessary
Fagron	Econazole nitrate	12I06-B40-306925	40	AR-16-FG-011359-01
Fagron	Econazole nitrate	12H08-N02	40	1312442
Fagron	Econazole nitrate	14G22-B07-327805	40	not necessary
Fagron	Econazole nitrate	11F09-N16	40	not necessary
Fagron	Enalapril maleate	17J18-B03-347278	40	not necessary
Fagron	Enalapril maleate	16K14-B02-336220	40	1801425
Fagron	Ethyl hydrogen f...	14C12-B07-292760	60	1410436
Fagron	Ethyl hydrogen f...	14C12-B07-292760	60	not necessary
Fagron	Fentanyl citrate	15F18-B01-525166	20	1316Q-03686
Fagron	Fentanyl citrate	15F18-B01-525098	20	1316R-03686
Fagron	Fentanyl citrate	16E26-B01-525360	40	2017A-03686
Fagron	Fentanyl citrate	15F18-B01-525166	20	1316Q-03686
Fagron	Fentanyl citrate	16E26-B01-525360	40	2017A-03686
Fagron	Fentanyl citrate	13G30-N06	20	0814M-07678
Fagron	Fentanyl citrate	15F18-B01-525098	20	1316R-03686
Fagron	Homatropine hydr...	18L11-B03-356938	40	20190122

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Supplier	Substance	Batch	Spectra	Certificate
Fagron	Hydromorphone hy...	13I25-N05	20	1516I-01334
Fagron	Hydromorphone hy...	13E16-N02	20	0914B-01334
Fagron	Hydromorphone hy...	15L08-B08-316877	40	1917Q-01334
Fagron	Hydromorphone hy...	13I25-N05	20	1516I-01334
Fagron	Indigo carmine	13K12-N01	40	1601099
Fagron	Macrogols 6000 p...	14C11-B01-296014	60	not necessary
Fagron	Macrogols 6000 p...	14J17-B01-309247	60	not necessary
Fagron	Macrogols 6000 p...	14J17-B01-309247	60	AR-16-FG-011486-01
Fagron	Magnesium aspart...	15I24-B89-313231	60	not necessary
Fagron	Magnesium aspart...	17C21-B05-333111	40	not necessary
Fagron	Magnesium aspart...	18D23-B01-350069	40	not necessary
Fagron	Magnesium aspart...	15I24-B89-313231	60	AR-16-FG-008660-03
Fagron	Methadone hydroc...	15E29-B02-313098	20	1516B-02949
Fagron	Methadone hydroc...	16F24-B02-323183	40	1917Q-02949
Fagron	Methadone hydroc...	15E29-B02-313098	20	1516B-02949
Fagron	Methadone hydroc...	13J24-B06	20	0914F-02949
Fagron	Methylosanilini...	13G03-N11	40	not necessary
Fagron	Methylosanilini...	13H28-N03	60	AR-15-FG-004742-01
Fagron	Methylosanilini...	13H28-N03	60	not necessary
Fagron	Midazolam	14C12-B31-313222	20	1516A-07393
Fagron	Midazolam	14C12-B31-313222	20	1516A-07393
Fagron	Midazolam	13K05-N01	20	0914E-07393
Fagron	Midazolam	16J03-B09-326963	40	1917Q-07393
Fagron	Midazolam	16J03-B09-326963	30	1917Q-07393
Fagron	Midazolam hydroc...	15H04-B03-314396	30	1917R-03538
Fagron	Midazolam hydroc...	14L23-B04-300245	20	1516A-03538
Fagron	Midazolam hydroc...	13E22-N09	20	0914F-03538
Fagron	Midazolam hydroc...	15J07-B01-320717	30	1917Q-03538
Fagron	Midazolam hydroc...	15J07-B01-320717	40	1917Q-03538
Fagron	Midazolam hydroc...	14L23-B04-300245	20	1516A-03538
Fagron	Morphine hydroch...	13G08-N04	20	0914G-01879
Fagron	Morphine hydroch...	16D21-B02-322088	40	1917Q-01879
Fagron	Morphine hydroch...	15I09-B08-312694	20	1416Q-01879
Fagron	Morphine hydroch...	16D21-B02-322088	40	1917Q-01879
Fagron	Morphine hydroch...	15I09-B08-312694	20	1416Q-01879
Fagron	Morphine sulfate	14F02-B06-315405	40	1917Q-07776
Fagron	Morphine sulfate	14F02-B06-315405	40	1917Q-07776
Fagron	Morphine sulfate	13J07-N04	20	0914G-07776
Fagron	Nitrofurantoin	11K-21-N23	40	not necessary
Fagron	Nitrofurantoin	15J15-B06-315225	60	not necessary
Fagron	Nitrofurantoin	12C30-N03	40	1401461
Fagron	Nitrofurantoin	15J15-B06-315225	60	AR-16-FG-003763-01
Fagron	Nitrofurantoin	12C30-N03	40	not necessary
Fagron	Nitrofurantoin	11I07-N11	40	not necessary
Fagron	Nitrofurantoin	13B28-N07	40	not necessary
Fagron	Phenobarbital	16G20-B04-328344	40	2017B-01040
Fagron	Phenobarbital	15G07-B06-311718	20	1416Q-01040
Fagron	Phenobarbital	16G20-B04-328344	40	2017B-01040
Fagron	Phenobarbital	15G07-B06-311718	20	1416Q-01040
Fagron	Prednisolone 1:1...	16F09-B04-341023	40	not necessary
Fagron	Rutoside trihydr...	13K12-B06-295483	60	not necessary
Fagron	Salbutamol sulfate	13K12-N02	40	not necessary
Fagron	Salbutamol sulfate	13K12-N02	40	1801521
Fagron	Salbutamol sulfate	13K12-N02	40	not necessary
Fagron	Salbutamol sulfate	13K12-N02	40	not necessary
Fagron	Salbutamol sulfate	13K12-N02	40	not necessary
Fagron	Salbutamol sulfate	13K12-N02	60	not necessary
Fagron	Salbutamol sulfate	17I21-B02	40	not necessary
Fagron	Salbutamol sulfate	13K12-N02	40	not necessary
Fagron	Silver protein a...	18000970	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Fagron	Sodium alginate	14G22-B99-297091	60	not necessary
Fagron	Sodium hydroxide...	12E02-N15	80	not necessary
Fagron	Thiamine nitrate	15A30-B06-309069	60	AR-16-FG-005855-01
Fagron	Thiomersal	11K01-N03	40	1401417
Fagron	Zinc orotate dihydrochloride	13J08-N05	40	not necessary
Galke	Blackberry leaf, cut	18060	40	not necessary
Galke	Boldo leaf, cut	19855	40	not necessary
Galke	Hawthorn leaf with fruit	21126	40	not necessary
Galke	Liquorice root, cut	22728	40	from supplier
Galke	Maté leaf, cut	21684	40	from supplier
Galke	Melissa leaf, cut	22218	40	from supplier
Galke	Nettle leaf, cut	21238	40	from supplier
Galke	Peppermint leaf, cut	19537	40	not necessary
Galke	Peppermint leaf, cut	20244	40	not necessary
Galke	Silverweed, cut	22840	40	not necessary
Galke	Thyme, rubbed	21932	40	not necessary
Gatt-Koller	Caffeine citrate	1783/05140715	60	AR-15-FG-014994-01
Gatt-Koller	Caffeine citrate	4065/11164916	40	not necessary
Inresa	Baclofen	206031617/09062017	40	AR-17-FG-018577-01
Inresa	Ketoprofen	F1300182	60	not necessary
Inresa	Ketoprofen	F1300183	60	AR-15-FG-009572-01
Inresa	Maltodextrin	R1600014	60	not necessary
Inresa	Maltodextrin	R1503902	60	AR-15-FG-008821-01
Inresa	Sotalol hydrochloride	369-MC	40	not necessary
Klenk	Agarikon	1061A120312	40	pending
Klenk	Angelica root	6085B120614	40	not necessary
Klenk	Angelica root	6085B120614	60	1509356
Klenk	Aniseed	2700A140129	60	not necessary
Klenk	Aniseed	2700A160511	60	1708049
Klenk	Ash bark, cut	0871B110127	60	not necessary
Klenk	Asparagus root, cut	6151B110304	40	1403480
Klenk	Birch bark, cut	0561A121121	40	not necessary
Klenk	Bitter fennel	2880N120418	40	AR-15-FG-002805-02
Klenk	Bitter fennel	2880N120418	40	1412547
Klenk	Bitter fennel	2860A140613	60	AR-15-FG-008160-01
Klenk	Black mustard seed	7430A120813	40	AR-15-FG-001050-01
Klenk	Black mustard seed	7434A120712	40	AR-15-FG-006711-01
Klenk	Boldo leaf, cut	1911A100714	40	not necessary
Klenk	Buckwheat seed	7510A111011	60	pending
Klenk	Buckwheat seed	7510A111011	40	from supplier
Klenk	Calendula flower	1241B130321	40	not necessary
Klenk	Cardamom, excorticated	2765A130524	60	AR-15-FG-015285-01
Klenk	Celery fruit	7140A130625	40	1405177
Klenk	Celery fruit	7140A131122	60	not necessary
Klenk	Celery root, cut	6091A110110	40	1410177
Klenk	Chelidonium majus	3731K120904	40	not necessary
Klenk	Chervil, rubbed	3721A100329	40	not necessary
Klenk	Cleavers goosegrass	4731B110809	40	not necessary
Klenk	Clove	1260A150916	40	1708050
Klenk	Clove, powdered	1264B141007	60	AR-15-FG-014858-01
Klenk	Comfrey root	6244B130624	40	not necessary
Klenk	Cottonwood bud, cut	3266B130826	40	1410178
Klenk	Cottonwood bud, cut	3266B150624	60	not necessary
Klenk	Cumin, powdered	2824B121001	40	not necessary
Klenk	Dandelion root, cut	6621B151029	60	AR-17-FG-007535-01
Klenk	Dill fruit	2680A170222	60	not necessary
Klenk	Elder berries	3010A120202	40	pending
Klenk	Elder leaf, cut	2321B130221	60	not necessary
Klenk	Elecampane rhizome	6341B120611	40	not necessary
Klenk	Euphrasy herb, cut	3871B100713	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Klenk	Fenugreek, powde...	7264A151001	60	AR-16-FG-014493-01
Klenk	Fenugreek, powde...	7264B130205	40	1408080
Klenk	Galeopsis herb, ...	3911A090219	40	not necessary
Klenk	Ginger, peeled, ...	6954B140724	60	AR-15-FG-014915-01
Klenk	Ginger, peeled, ...	6954B150325	60	1606616
Klenk	Ginger, peeled, ...	6954B170127	60	1708675
Klenk	Ginger, peeled, ...	6954B160429	60	1704440
Klenk	Goat's rue, cut	3901C110905	40	not necessary
Klenk	Greek mountain h...	4511K130314	40	not necessary
Klenk	Green tea	5100A100611	40	not necessary
Klenk	Hay flower	1400A130304	40	not necessary
Klenk	Java tea, cut	2221B110718	40	not necessary
Klenk	Juniper, powdered	2894B150922	60	1704439
Klenk	Juniper, powdered	2894B130320	40	1411362
Klenk	Knotgrass, cut	4301A120912	40	not necessary
Klenk	Ladys bedstraw ...	3921B101012	40	not necessary
Klenk	Laurel leaf, pow...	2124A110329	40	1411032
Klenk	Laurel leaf, pow...	2124A110329	60	not necessary
Klenk	Maize style, cut	5581A111206	40	not necessary
Klenk	Meadowsweet herb...	4541A120313	60	not necessary
Klenk	Melissa leaf, cut	2161A090630	130	not necessary
Klenk	Melissa leaf, cut	2161A121029	55	not necessary
Klenk	Motherwort herb,...	4071A121211	40	not necessary
Klenk	Myrrh	3355B120628	40	AR-15-FG-000945-01
Klenk	Nettle seed	7470A111117	40	pending
Klenk	Nutmeg	7320A121002	40	not necessary
Klenk	Nutmeg, powdered...	7325A160405	60	9888
Klenk	Parsley herb, ru...	4262A091116	60	not necessary
Klenk	Parsley seed	7370A130909	40	1407600
Klenk	Passionflower he...	4231A120329	40	not necessary
Klenk	Peony root, cut	6421B120327	60	not necessary
Klenk	Restharrow root,...	6411B130404	40	not necessary
Klenk	Rose hips seed	7240A120402	60	not necessary
Klenk	Rosemary leaf, cut	2261A131118	60	AR-15-FG-008499-01
Klenk	Ruscus rhizome, ...	7081B110301	60	not necessary
Klenk	Saffron (spice)	0384A121022	40	not necessary
Klenk	Senna leaf, powd...	2334B130606	60	AR-15-FG-015212-01
Klenk	Strawberry leaf,...	2031B110224	40	not necessary
Klenk	Strawberry leaf,...	2031B120925	40	not necessary
Klenk	Sweet fennel	2870A110412	40	pending
Klenk	Sweet fennel	2870A130304	40	1405154
Klenk	Theriac, powdered	13816	60	1705088
Klenk	Tormentil	6914B120112	40	not necessary
Klenk	Tormentil	6911B141114	60	AR-15-FG-014020-01
Klenk	Verbena herb, cut	4651B120611	40	not necessary
Klenk	Willowherb, smal...	4721A140203	60	not necessary
Kräuter Schulte	Twotoothed achyr...	45053	40	not necessary
Kreatin.de GmbH	Creatine	300331	50	1405615
Lycored corp.	Caromix	CMX-LLCV-011401	40	not necessary
Merck KGaA	Benzoyl peroxide...	S7012241509	60	20130317
Otto Fischar	Talcum	90841/1	40	from supplier
Pharmorgana	L-carnitine tart...	1000170113	40	from supplier
Pharmorgana	L-carnitine tart...	1000160672	40	from supplier
Pharmorgana	Sodium dichloroa...	1000150016	40	from supplier
Roth	Brilliant blue R...	314217301	60	from supplier
Roth	Deoxycholic acid...	154212633	60	not necessary
Roth	Deoxycholic acid...	385212633	60	not necessary
Roth	Deoxycholic acid...	084181622	40	1405618
Roth	Esculin	155206581	60	not necessary
Roth	Theobromine, 99%	145191010	60	AR-16-FG-002141-01

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Supplier	Substance	Batch	Spectra	Certificate
Roth	Theobromine, 99%	365191010	60	not necessary
Roth	Trypan blue (C.I...	204209355	60	from supplier
Safic-Alcan	Amygdalin, bitte...	BAE150902	20	from supplier
Safic-Alcan	Amygdalin, bitte...	BAE150902	20	from supplier
Safic-Alcan	Dimercaptosuccin...	20180130	40	from supplier
Sand 12 GmbH	D-ribose	L201211720	35	not necessary
Sigma-Aldrich	Bromelain	BCBM1589V	40	not necessary
Sigma-Aldrich	Bromothymol blue	MKBQ5404V	40	pending
Spinnrad	Inulin	1112300433	40	not necessary
Th. Geyer	Amphetamine sulf...	067043	40	2017C-03361
Th. Geyer	Amphetamine sulf...	067043	40	2017C-03361
Th. Geyer	Amphetamine sulf...	67002	20	0814I-03361
Th. Geyer	Calcium colamine...	33299	20	from supplier
Th. Geyer	Calcium colamine...	36986	40	from supplier
Th. Geyer	Cocaine hydrochl...	60145	20	0814K-01278
Th. Geyer	Codeine phosphat...	67038	20	0814K-01279
Th. Geyer	Codeine phosphat...	067054	40	2017D-01279
Th. Geyer	Codeine phosphat...	067054	40	2017D-01279
Th. Geyer	Dihydrocodeine h...	067052	40	2017D-03065
Th. Geyer	Dihydrocodeine h...	67035	20	0914D-03065
Th. Geyer	Methadone hydroc...	067055	40	1917S-02949
Th. Geyer	Methadone hydroc...	67047	20	0914H-02949
Th. Geyer	Methadone hydroc...	67033	20	0914G-02949
Th. Geyer	Methadone hydroc...	067055	40	1917S-02949
Th. Geyer	Mg-Ca-K colamine...	54610	40	from supplier
Th. Geyer	Mg-Ca-K colamine...	36985	20	from supplier
Th. Geyer	Mg-Ca-K colamine...	54610	40	from supplier
Th. Geyer	Morphine hydroch...	67036	20	0914H-01879
Th. Geyer	Phenobarbital	67045	20	0914F-01040
Th. Geyer	Phenobarbital	067056	40	2017A-01040
VMP Chemiekon...	D-(+)-glucosamin...	144212943	40	20140402
Yino Pharma	Sodium chondroit...	YN010511805005	40	not necessary
Yino Pharma	Sodium chondroit...	YN010511806007	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 7075 batches. From these, 15 969 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
A.H. 27.05.13 ek: 6,75EUR	Male speedwell wort, ...	274239	1
AHD	Bitter fennel	15006502	1
AHD	Sodium monohydrogenph...	112345013	1
AHD	Tragacanth, powdered	15379906	3
AHD 10.02.17 EK.3,50	Aniseed	16200801	3
AHD;11.05.15;3,23	Bitter fennel	14376408	3
Akazie	Black cumin seed	20.09.2015	1
Akazie	Cinnamon, cut	20.09.2015	1
Akazie	Dill fruit	20.09.2015	1
Akazie	Linseed	20.09.2015	2
Akazie	Rosemary leaf, cut	20.09.2015	1
Akazien-Apo	Cinnamon, cut	Test	1
Aldrich	Sodium propionate	U02796-056	1
Alfred Galke	Alchemilla, cut	20921	1
Alfred Galke	Bitter fennel	18270	1
Alfred Galke	Caraway fruit	20069	1
Alfred Galke	Melissa leaf, cut	D-NI-1-9516-BC	1
Alfred Galke	Raspberry leaf, cut	19851	1
Alfred Galke	Shepherd's purse, cut	20591	1
Alfred Galke	Yarrow herb, cut	19861	1
Alliance	Agrimony, cut	11374004	5
Alliance	Hawthorn flower	13010403	1
Alliance	Heather, cut	255389	1
Alliance	Sodium hydrogen carbo...	12324704	1
Alliance	Sodium monohydrogenph...	12256606	1
Alliance Health	Aluminium potassium s...	13025401	3
Alliance healthcare	Sodium monohydrogenph...	12L05-N04	2
Alliance Healthcare	Aluminium potassium s...	13025404	1
Allianz Healthcare	Pumpkin seed, peeled	16081210	1
Alte Apotheke	Oak bark, cut	15314904	2
an	Blessed thistle, cut	13389704	1
an	Gentian root, cut	6311b130305	1
an	Hawthorn leaf with fl...	1971A130930	2
an	Passionflower herb, cut	13141212	1
an	Raspberry leaf, cut	13086708	1
an	Roselle	14018101	1
an	Verbena herb, cut	12383007	1
Anzag	Aluminium chloride he...	1204026-02	15
Anzag	Aluminium potassium s...	1218441	1
Anzag	Bilberry fruit, dried	2910N120921	2
Anzag	Blackberry leaf, cut	10136412	1
Anzag	Blessed thistle, cut	282281	1
Anzag	Calendula flower, cut	12221706	12
Anzag	Dandelion herb with r...	274030	1
Anzag	Ispaghula seed	11185818	1
Anzag	Lavender flower	1488A12803	1

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Supplier	Substance	Batch	Spectra
Anzag	Linseed	12137105	1
Anzag	Magnesium chloride he...	1304003-01	2
Anzag	Magnesium chloride he...	120802501	1
Anzag	Magnesium sulfate hep...	204035	1
Anzag	Maize style, cut	274920	1
Anzag	Meadowsweet herb, cut	10381604	5
Anzag	Nettle leaf, cut	2381-A130122	1
Anzag	Passionflower herb, cut	1207211669	1
Anzag	Raspberry leaf, cut	2291A120806	2
Anzag	Raspberry leaf, cut	12103107	10
Anzag	Sweet woodruff herb, ...	12103504	2
Anzag	Trichloroacetic acid	12135204	2
ANZAG	Walnut leaf, cut	12124603	10
Anzag 05.12.12	Agrimony, cut	11374002	3
Anzag 06.04.2016	Aniseed	15398601	1
Anzag 10.05.13 ek:3,16EUR	Dandelion herb with r...	6611B130321	1
Anzag 12.03.13 ek: 4,...	St. John's wort, cut	11185608	2
Anzag 12.11.12 ek:3,85	Yarrow herb, cut	11280513	1
Anzag 17.04.13 ek: 2,...	Tall golden rod, cut	4521A110816	2
Anzag 22.03.13 ek: 5,...	Aloes, cape, powdered	12232102	1
Anzag 25.10.12 ek:3.16EUR	Dandelion herb with r...	6611B110131	1
Anzag 26.10.12 2.36EUR	Oak bark, cut	10348616	6
Anzag 27.12.12 ek:2,79	Blackberry leaf, cut	10136048	1
Anzag 29.04.13 ek: 4,...	Magnesium sulfate hep...	12138518	3
Anzag ek: 15,60 20.07...	Iceland moss, cut	11101605	1
Anzag ek: 2,59EUR 19.09...	Caraway fruit	11003216	3
Anzag ek: 3,06 11.09...	Sage leaf, cut	2301A120403	36
Anzag ek: 4,58EUR 25.09...	Walnut leaf, cut	2111A120123	8
Anzag ek: 4,88EUR 26.09...	Male speedwell wort, ...	4661C120321	10
Anzag ek: 6,39 11.09...	Alchemilla, cut	11182806	6
Anzag ek:2,50EUR 15.09.12	Horse chestnut leaf, ...	2551B111013	7
Anzag ek:2,64EUR 16.07.12	Mistletoe, cut	10273417	1
Anzag ek:3,00EUR 11.09.12	Raspberry leaf, cut	12103105	18
Anzag ek:3,13EUR 15.09.12	Melilot herb, cut	11307605	4
Anzag ek:8.77EUR 30.08.12	Manna, cut	11308904	2
Anzag EK4,31 17.08.12	Nettle leaf, cut	2381A110913	19
Anzag EK7,91 08.08.12	Gentian root, cut	10263407	1
Anzag/ Hedinger	Sodium hydrogen carbo...	206027	1
Apofit	Blue bottle flower wi...	278776	1
Apofit	Fenugreek	222392	1
ApoFit/Noweda	Walnut leaf, cut	271137	1
Apomix	Trichloroacetic acid	12G04-M11	1
Apomix / 11	Carbachol	12330703	1
Apotheke Bühlau	Almonds, bitter, whole	267467	2
Apotheke Bühlau	Horse chestnut leaf, ...	100416	1
Aurica	Aniseed	521302895	1
Aurica	Birch leaf, cut	521205644	1
Aurica	Common wormwood herb,...	521305386	1
Aurica	Dandelion herb with r...	521200197	1
Aurica	Red clover flower	521206331	1
Aurica	Red clover flower	521203442	1
Aurica	Rose hips with peel, ...	521201801	1
Aurica	Sage leaf, cut	521204613	1
Aurica	St. John's wort, cut	521202559	1
Aurica	St. John's wort, cut	521200778	1
Aurica	Tall golden rod, cut	224133	1
Aurica	Tall golden rod, cut	521201267	1
Aurica	Thyme, rubbed	521207003	1
Aurica	Valerian root, cut	221838	2
Aurica	Verbena herb, cut	521305668	1

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Supplier	Substance	Batch	Spectra
Aurica / 11	Equisetum stem, cut	521302898	1
Aurica / 11	Juniper	521301390	1
Aurica / 11	Primrose flower	521301234	1
Aurica Naturheilmitte...	Aniseed, powdered	521405796	1
Aurica/Anzag	Red clover flower	521303918	1
Aurica/Gehe	Primrose flower	521203308	1
aurica/phoenix	Liquorice root, natur...	521206925	1
Aurica/Phönix	Acorus root, peeled	150649	1
Aurica/Phönix	Angelica root	520800638	1
Aurica/Phönix	Bean shells, cut	5052301	1
Aurica/Phönix	Centaury, cut	520702152	1
Aurica/Phönix	Juniper	521006043	1
Aurica/Phönix	Maize style, cut	520901387	1
Aurica/Phönix	Male speedwell wort, ...	520708362	1
Aurica/Phönix	Mistletoe, cut	6110801	1
Bahnhof-Apotheke	Acorus root, peeled	17-121107	1
Bahnhof-Apotheke	Alchemilla, cut	17-121107	1
Bahnhof-Apotheke	Aniseed	7-120913	1
Bahnhof-Apotheke	Birch leaf, cut	18-120702	1
Bahnhof-Apotheke	Bitter fennel	11-121029	1
Bahnhof-Apotheke	Blackberry leaf, cut	18-120702	1
Bahnhof-Apotheke	Calendula flower, cut	17-121106	1
Bahnhof-Apotheke	Caraway fruit	18-120709	1
Bahnhof-Apotheke	Elder flower, rubbed	17-121112	1
Bahnhof-Apotheke	Hawthorn leaf with fl...	7-121011	1
Bahnhof-Apotheke	Hay flower	13-121105	1
Bahnhof-Apotheke	Lime flower, cut	7-121011	1
Bahnhof-Apotheke	Liquorice root, peeled	17-121112	1
Bahnhof-Apotheke	Lycopodium herb, cut	17-121112	1
Bahnhof-Apotheke	Maize style, cut	20-121018	1
Bahnhof-Apotheke	Male speedwell wort, ...	4-121002	1
Bahnhof-Apotheke	Matricaria flower	11-121024	1
Bahnhof-Apotheke	Melissa leaf, cut	17-120917	1
Bahnhof-Apotheke	Nettle leaf, cut	7-121109	1
Bahnhof-Apotheke	Oak bark, cut	17-121106	1
Bahnhof-Apotheke	Psyllium seed	3-121005	1
Bahnhof-Apotheke	Raspberry leaf, cut	17-120917	1
Bahnhof-Apotheke	Ribwort plantain, cut	7-121011	1
Bahnhof-Apotheke	Rosemary leaf, cut	7-120915	1
Bahnhof-Apotheke	Sage leaf, cut	3-121018	1
Bahnhof-Apotheke	Shepherd's purse, cut	4-120924	1
Bahnhof-Apotheke	St. John's wort, cut	4-121018	1
Bahnhof-Apotheke	Thyme, rubbed	17-121112	1
Bahnhof-Apotheke	Willowherb, small flo...	17-121107	1
Bahnhof-Apotheke	Wormwood herb, cut	17-121107	1
Bahnhof-Apotheke	Yarrow herb, cut	7-121011	1
Berkel AHK	Agnus castus fruit	14194401	4
Berkel AHK	Aniseed	11374103	1
Berkel AHK	Aniseed	14194401	1
Berkel AHK	Oak bark, cut	13360310	1
Berkel AHK	Valerian root, powdered	14179403	2
Berkel AHK	Valerian root, powdered	13287406	1
BLS	Phenobarbital	67056	2
bohn	Savory, rubbed	12177208	1
Bomastus-Werke/Phönix	Rosemary leaf, cut	298424	2
Bomba/AHD	Equisetum stem, cut	280449	3
Bomba/AHD	Senna leaf, cut	280008	1
Bomba/AHD	Tall golden rod, cut	279526	1
Bomba/AHD	Willow bark, cut	280362	1
Bombaltus	Hop strobile	274724	1

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Supplier	Substance	Batch	Spectra
Bombastus	Acorus root, natural,...	277958	1
Bombastus	Acorus root, natural,...	224114	1
Bombastus	Acorus root, natural,...	274159	1
Bombastus	Acorus root, natural,...	276260	2
Bombastus	Acorus root, natural,...	281692	1
Bombastus	Acorus root, peeled	274159	3
Bombastus	Acorus root, peeled	267365	1
Bombastus	Alchemilla, cut	278889	1
Bombastus	Alchemilla, cut	279070	4
Bombastus	Alchemilla, cut	276173	3
Bombastus	Alchemilla, cut	521203995	1
Bombastus	Alchemilla, cut	266404	1
Bombastus	Alchemilla, cut	272021	5
Bombastus	Alchemilla, cut	14066007	1
Bombastus	Alchemilla, cut	282032	1
Bombastus	Alchemilla, cut	231013B	1
Bombastus	Almonds, bitter, whole	306048	1
Bombastus	Almonds, bitter, whole	1700352	2
Bombastus	Almonds, bitter, whole	305322	2
Bombastus	Almonds, bitter, whole	304961	1
Bombastus	Almonds, bitter, whole	297921	1
Bombastus	Almonds, bitter, whole	267529	1
Bombastus	Almonds, bitter, whole	275600	1
Bombastus	Almonds, bitter, whole	275001	2
Bombastus	Almonds, bitter, whole	284978	1
Bombastus	Almonds, bitter, whole	275601	1
Bombastus	Almonds, bitter, whole	283369	1
Bombastus	Almonds, bitter, whole	303218	2
Bombastus	Angelica root	281280	7
Bombastus	Angelica root	278757	4
Bombastus	Angelica root	272895	1
Bombastus	Angelica root	270117	1
Bombastus	Angelica root	274128	2
Bombastus	Angelica root	275878	1
Bombastus	Angelica root	291848	1
Bombastus	Angelica root	290309	1
Bombastus	Angelica root	305460	1
Bombastus	Angelica root	307041	3
Bombastus	Angelica root	296334/1121115	1
Bombastus	Angelica root	272954	1
Bombastus	Angelica root	301768	1
Bombastus	Angelica root	295085	2
Bombastus	Angelica root	278294	1
Bombastus	Angelica root	275879	1
Bombastus	Angelica root	269775	2
Bombastus	Aniseed	285777	1
Bombastus	Aniseed	282917	2
Bombastus	Aniseed	289846	2
Bombastus	Aniseed	305177	1
Bombastus	Aniseed	285778	2
Bombastus	Artichoke leaf, cut	8202213593	1
Bombastus	Bean shells, cut	278696	2
Bombastus	Bean shells, cut	272781	3
Bombastus	Bean shells, cut	270517	1
Bombastus	Bean shells, cut	240503	1
Bombastus	Bean shells, cut	278686	1
Bombastus	Bean shells, cut	282475	1
Bombastus	Bearberry leaf, cut	267926	1
Bombastus	Bearberry leaf, cut	272297	8
Bombastus	Bearberry leaf, cut	275491	2

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Supplier	Substance	Batch	Spectra
Bombastus	Betony herb, cut	12007205	2
Bombastus	Bilberry leaf, cut	272176	2
Bombastus	Birch leaf, cut	267077	1
Bombastus	Birch leaf, cut	270743	1
Bombastus	Birch leaf, cut	272385	1
Bombastus	Birch leaf, cut	287280	1
Bombastus	Birch leaf, cut	280677	1
Bombastus	Bitter fennel	275922	4
Bombastus	Bitter fennel	280891	2
Bombastus	Bitter fennel	285609	1
Bombastus	Bitter fennel	289870	2
Bombastus	Bitter fennel	289869	2
Bombastus	Bitter fennel	289870	1
Bombastus	Bitter fennel	296877	3
Bombastus	Bitter fennel	293627	1
Bombastus	Bitter fennel	299386	3
Bombastus	Bitter fennel	299385	2
Bombastus	Bitter fennel	268130	2
Bombastus	Bitter orange peel, cut	274240	3
Bombastus	Bitter orange peel, cut	278233	4
Bombastus	Blackberry leaf, cut	267122	1
Bombastus	Blackberry leaf, cut	273668	2
Bombastus	Blue bottle flower wi...	284030	1
Bombastus	Blue bottle flower wi...	275759	2
Bombastus	Calendula flower	268626	1
Bombastus	Calendula flower	280306	1
Bombastus	Calendula flower, cut	275813	1
Bombastus	Calendula flower, cut	275128	1
Bombastus	Calendula flower, cut	207294	1
Bombastus	Calendula flower, cut	234997	1
Bombastus	Calendula flower, cut	270046	1
Bombastus	Calendula flower, cut	253620	1
Bombastus	Caraway fruit	270124	1
Bombastus	Caraway fruit	282269	1
Bombastus	Caraway fruit	275849	1
Bombastus	Centaury, cut	277598	3
Bombastus	Coltsfoot leaf, cut	269501	3
Bombastus	Coltsfoot leaf, cut	285263	3
Bombastus	Coltsfoot leaf, cut	277131	1
Bombastus	Coltsfoot leaf, cut	281100	4
Bombastus	Coltsfoot leaf, cut	232339	1
Bombastus	Coltsfoot leaf, cut	278758	7
Bombastus	Coltsfoot leaf, cut	277848	2
Bombastus	Coltsfoot leaf, cut	276303	5
Bombastus	Coltsfoot leaf, cut	272019	1
Bombastus	Coltsfoot leaf, cut	275489	3
Bombastus	Coltsfoot leaf, cut	274289	5
Bombastus	Coltsfoot leaf, cut	265856	1
Bombastus	Comfrey herb, cut	281531	1
Bombastus	Coriander	263733	1
Bombastus	Couch grass rhizome, ...	273387	3
Bombastus	Couch grass rhizome, ...	262175	1
Bombastus	Couch grass rhizome, ...	270500	1
Bombastus	Couch grass rhizome, ...	276777	3
Bombastus	Dandelion herb with r...	290125	1
Bombastus	Dandelion herb with r...	282916	7
Bombastus	Dandelion herb with r...	280363-3385310110	1
Bombastus	Dandelion herb with r...	280363	5
Bombastus	Dandelion herb with r...	285264	1
Bombastus	Dandelion herb with r...	277597	6

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Supplier	Substance	Batch	Spectra
Bombastus	Dandelion herb with r...	275126	1
Bombastus	Dandelion herb with r...	274030	4
Bombastus	Dandelion herb with r...	258809	1
Bombastus	Dandelion herb with r...	271272	5
Bombastus	Dill herb, cut	50836505	1
Bombastus	Elder flower, rubbed	269873	2
Bombastus	Elder flower, rubbed	275393	4
Bombastus	Elder flower, rubbed	265631	1
Bombastus	Elder flower, rubbed	279216	3
Bombastus	Equisetum stem, cut	6011401	1
Bombastus	Equisetum stem, cut	18111304	1
Bombastus	Equisetum stem, cut	268321	1
Bombastus	Equisetum stem, cut	280647	1
Bombastus	Equisetum stem, cut	265924	1
Bombastus	Equisetum stem, cut	275891	3
Bombastus	Equisetum stem, cut	264100	1
Bombastus	Equisetum stem, cut	272552	2
Bombastus	Equisetum stem, cut	273963	1
Bombastus	Equisetum stem, cut	264101	1
Bombastus	Equisetum stem, cut	274714	1
Bombastus	Equisetum stem, cut	278107	1
Bombastus	Euphrasy herb, cut	278108	2
Bombastus	Euphrasy herb, cut	277846	1
Bombastus	Euphrasy herb, cut	274553	1
Bombastus	Frangula bark, cut	275998	2
Bombastus	Frangula bark, cut	238812	1
Bombastus	Frangula bark, cut	278599	3
Bombastus	Frangula bark, cut	281284	2
Bombastus	Frangula bark, cut	273926	1
Bombastus	Frangula bark, cut	270733	1
Bombastus	Frangula bark, cut	268407	1
Bombastus	Ginseng root	13150903	1
Bombastus	Hawthorn leaf with fl...	273287	1
Bombastus	Hawthorn leaf with fl...	275310	2
Bombastus	Hawthorn leaf with fl...	267000	1
Bombastus	Hawthorn leaf with fl...	267551	1
Bombastus	Hawthorn leaf with fl...	264044	1
Bombastus	Hawthorn leaf with fl...	272881	1
Bombastus	Hawthorn leaf with fl...	278756	1
Bombastus	Heather, cut	278314	1
Bombastus	Hop strobile	208502	1
Bombastus	Hop strobile	276976	1
Bombastus	Hop strobile	271870	1
Bombastus	Iceland moss, cut	13357802	1
Bombastus	Lavender flower	279213	1
Bombastus	Lavender flower	274469	1
Bombastus	Lime flower, cut	280678	3
Bombastus	Lime flower, cut	275129	2
Bombastus	Linseed	269500	1
Bombastus	Linseed	274032	1
Bombastus	Linseed	295376	1
Bombastus	Linseed	278457	6
Bombastus	Linseed	282734	3
Bombastus	Linseed	1610	1
Bombastus	Liquorice root, peeled	270192	1
Bombastus	Liquorice root, peeled	268001	1
Bombastus	Liquorice root, natur...	2901312151	1
Bombastus	Liquorice root, natur...	286584	1
Bombastus	Liquorice root, natur...	285185	2
Bombastus	Liquorice root, natur...	3713Q2151	1

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Supplier	Substance	Batch	Spectra
Bombastus	Liquorice root, natur...	5091305	1
Bombastus	Liquorice root, natur...	279409	1
Bombastus	Liquorice root, natur...	278377	3
Bombastus	Liquorice root, natur...	903312151	1
Bombastus	Liquorice root, natur...	276468	6
Bombastus	Liquorice root, natur...	274921	3
Bombastus	Lovage root, cut	273001	1
Bombastus	Magnesium sulfate hep...	277424	1
Bombastus	Maize style, cut	282574	1
Bombastus	Maize style, cut	81113a	1
Bombastus	Maize style, cut	276776	1
Bombastus	Maize style, cut	285912	1
Bombastus	Male speedwell wort, ...	274238	1
Bombastus	Mallow flower, cut	13267304	1
Bombastus	Marian thistle fruit	278379	1
Bombastus	Marian thistle fruit	296535	1
Bombastus	Marian thistle fruit	284420	1
Bombastus	Marian thistle fruit	13122013a	1
Bombastus	Marian thistle fruit	282034	2
Bombastus	Marian thistle fruit	299483	1
Bombastus	Marian thistle fruit	269499	1
Bombastus	Marian thistle fruit	279405	3
Bombastus	Marian thistle fruit	278378	1
Bombastus	Marian thistle fruit	277720	3
Bombastus	Marian thistle fruit	296193	1
Bombastus	Marshmallow root, nat...	270467	1
Bombastus	Marshmallow root, pee...	273458	1
Bombastus	Matricaria flower	268408	1
Bombastus	Matricaria flower	277959	2
Bombastus	Matricaria flower	281103	2
Bombastus	Matricaria flower	276307	1
Bombastus	Matricaria flower	264997	1
Bombastus	Matricaria flower	273667	1
Bombastus	Matricaria flower	283710	2
Bombastus	Matricaria flower	268712	1
Bombastus	Matricaria flower	276095	5
Bombastus	Matricaria flower	299185	1
Bombastus	Matricaria flower	287855	1
Bombastus	Matricaria flower	271781	1
Bombastus	Matricaria flower	265419	1
Bombastus	Matricaria flower	268408	1
Bombastus	Matricaria flower	274105	1
Bombastus	Matricaria flower	274106	1
Bombastus	Melissa leaf, cut	277722	1
Bombastus	Melissa leaf, cut	270044	1
Bombastus	Melissa leaf, cut	271499	2
Bombastus	Methadone hydrochloride	14C24-B01-292858	6
Bombastus	Mistletoe, cut	277432	2
Bombastus	Nettle leaf, cut	266638	1
Bombastus	Nettle leaf, cut	266099	1
Bombastus	Nettle leaf, cut	273229	2
Bombastus	Nettle leaf, cut	275848	3
Bombastus	Nettle leaf, cut	270854	3
Bombastus	Nettle leaf, cut	270987	2
Bombastus	Nettle leaf, cut	275763	1
Bombastus	Nettle leaf, cut	280305	2
Bombastus	Oak bark, cut	286297	1
Bombastus	Oak bark, cut	272704	1
Bombastus	Oak bark, cut	265717	1
Bombastus	Oak bark, cut	274611	1

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Supplier	Substance	Batch	Spectra
Bombastus	Oak bark, cut	279525	2
Bombastus	Oak bark, cut	274392	1
Bombastus	Oak bark, cut	229090	1
Bombastus	Peppermint leaf, cut	272956	3
Bombastus	Peppermint leaf, cut	278679	2
Bombastus	Peppermint leaf, cut	279634	1
Bombastus	Peppermint leaf, cut	279214	1
Bombastus	Peppermint leaf, cut	276514	1
Bombastus	Peppermint leaf, cut	281282	1
Bombastus	Peppermint leaf, cut	285914	1
Bombastus	Peppermint leaf, cut	271499	1
Bombastus	Peppermint leaf, cut	282509	1
Bombastus	Peppermint leaf, cut	281043	3
Bombastus	Peppermint leaf, cut	255719	1
Bombastus	Peppermint leaf, cut	246514	1
Bombastus	Peppermint leaf, cut	275295	3
Bombastus	Peppermint leaf, cut	266772	2
Bombastus	Peppermint leaf, cut	273843	2
Bombastus	Peppermint leaf, cut	279914	2
Bombastus	Raspberry leaf, cut	274507	1
Bombastus	Raspberry leaf, cut	273778	1
Bombastus	Raspberry leaf, cut	269870	1
Bombastus	Raspberry leaf, cut	248586	1
Bombastus	Raspberry leaf, cut	273668	2
Bombastus	Raspberry leaf, cut	272898	1
Bombastus	Raspberry leaf, cut	267122	1
Bombastus	Raspberry leaf, cut	279686	3
Bombastus	Restharrow root, cut	272831	2
Bombastus	Restharrow root, cut	274421	1
Bombastus	Restharrow root, cut	283708	1
Bombastus	Rhubarb, powdered	11043806	1
Bombastus	Ribwort plantain, cut	276453	1
Bombastus	Ribwort plantain, cut	275479	1
Bombastus	Rose hips peel, cut	257166	1
Bombastus	Rose hips peel, cut	285184	1
Bombastus	Rose hips peel, cut	231013A	1
Bombastus	Rose hips peel, cut	277431	3
Bombastus	Rose hips peel, cut	283458	1
Bombastus	Rose hips peel, cut	275394	2
Bombastus	Rosemary leaf, cut	277128	1
Bombastus	Rosemary leaf, cut	270171	1
Bombastus	Rosemary leaf, cut	281843	1
Bombastus	Rosemary leaf, cut	281248	1
Bombastus	Sage leaf, cut	270115	1
Bombastus	Sage leaf, cut	255381	1
Bombastus	Sage leaf, cut	277512	1
Bombastus	Sage leaf, cut	271253	1
Bombastus	Senna leaf, cut	280448	1
Bombastus	Senna leaf, cut	273547	3
Bombastus	Senna leaf, cut	273474	1
Bombastus	Senna leaf, cut	278109	1
Bombastus	Senna leaf, cut	280581	2
Bombastus	Shepherd's purse, cut	269594	3
Bombastus	Shepherd's purse, cut	278856	2
Bombastus	Shepherd's purse, cut	284136	1
Bombastus	Shepherd's purse, cut	12345	2
Bombastus	Shepherd's purse, cut	269977	1
Bombastus	Sodium monohydrogenph...	11H04-N06	1
Bombastus	St. John's wort, cut	265761	1
Bombastus	St. John's wort, cut	281530	1

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Supplier	Substance	Batch	Spectra
Bombastus	St. John's wort, cut	268834	2
Bombastus	St. John's wort, cut	275106	6
Bombastus	St. John's wort, cut	268913	1
Bombastus	Tall golden rod, cut	271460	1
Bombastus	Tall golden rod, cut	271459	1
Bombastus	Tall golden rod, cut	209974	1
Bombastus	Tall golden rod, cut	261756	1
Bombastus	Tall golden rod, cut	274290	1
Bombastus	Tall golden rod, cut	278697	2
Bombastus	Tall golden rod, cut	270047	2
Bombastus	Thyme, rubbed	277996	2
Bombastus	Thyme, rubbed	277466	1
Bombastus	Thyme, rubbed	273909	3
Bombastus	Thyme, rubbed	243485	1
Bombastus	Turmeric, javanese, cut	284242	2
Bombastus	Turmeric, javanese, cut	282221	2
Bombastus	Turmeric, javanese, cut	277130	1
Bombastus	Turmeric, javanese, cut	262792	1
Bombastus	Valerian root, cut	269457	1
Bombastus	Valerian root, cut	267863	1
Bombastus	Valerian root, cut	274722	1
Bombastus	Walnut bark, cut	711B1206130	1
Bombastus	Wild pansy, cut	282661	1
Bombastus	Wild pansy, cut	279314	3
Bombastus	Wild pansy, cut	278106	2
Bombastus	Wild pansy, cut	220232	1
Bombastus	Wild pansy, cut	276259	3
Bombastus	Wild pansy, cut	278106	1
Bombastus	Wild pansy, cut	272832	1
Bombastus	Wild pansy, cut	274237	2
Bombastus	Wild pansy, cut	280890	1
Bombastus	Willow bark, cut	261615	1
Bombastus	Willow bark, cut	251385	1
Bombastus	Willow bark, cut	277005	3
Bombastus	Willow bark, cut	278458	2
Bombastus	Willow bark, cut	277847	1
Bombastus	Willow bark, cut	161594	1
Bombastus	Willow bark, cut	282270	1
Bombastus	Willow bark, cut	288869	1
Bombastus	Willow bark, cut	281533	2
Bombastus	Willowherb, small flo...	281846	2
Bombastus	Wormwood herb, cut	265417	2
Bombastus	Wormwood herb, cut	281000	1
Bombastus	Wormwood herb, cut	221868	1
Bombastus	Yarrow herb, cut	276498	1
Bombastus	Yarrow herb, cut	274610	2
Bombastus	Yarrow herb, cut	274284	1
Bombastus	Yarrow herb, cut	15006702	1
Bombastus	Yarrow herb, cut	275964	1
C	Robert herb, cut	11147810	3
Caaelo	Sodium sulfate decahy...	11294603	2
Cae	Bean shells, cut	Int.Ch.313011	1
Cae	Bilberry fruit, dried	212172	1
Cae	Bitter fennel	Int.Ch.314090	1
Caelo	Abrotani herb, cut	2091305	1
Caelo	Acorus root, natural,...	284875	2
Caelo	Acorus root, natural,...	13127801	1
Caelo	Acorus root, natural,...	12066501	1
Caelo	Acorus root, peeled	12275604-3544411013	1
Caelo	Acorus root, peeled	12295903	1

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Supplier	Substance	Batch	Spectra
Caelo	Acorus root, peeled	6701B130103	19
Caelo	Acorus root, peeled	12066501	7
Caelo	Acorus root, peeled	12295901	1
Caelo	Acorus root, peeled	12066502	1
Caelo	Acorus root, peeled	7061302	1
Caelo	Acorus root, peeled	12056701	1
Caelo	Acorus root, peeled	12295902	4
Caelo	Acorus root, peeled	24081203	1
Caelo	Acorus root, peeled	12275604	2
Caelo	Acorus root, peeled	8031306	1
Caelo	Acorus root, peeled	15061202	1
Caelo	Acorus root, peeled	12275602	7
Caelo	Acorus root, peeled	12295904	4
Caelo	Acorus root, peeled	12239008	1
Caelo	Acorus root, peeled	13101306	1
Caelo	Acorus root, peeled	241013010	1
Caelo	Acorus root, peeled	28121205	1
Caelo	Acorus root, peeled	12056703	1
Caelo	Acorus root, peeled	313060	1
Caelo	Agarikon	11024502	1
Caelo	Agnus castus fruit	11026309	1
Caelo	Agnus castus fruit	12274010	10
Caelo	Agnus castus fruit	11026318	1
Caelo	Agnus castus fruit	15318718	1
Caelo	Agnus castus fruit	15318702	1
Caelo	Agnus castus fruit	15065105	1
Caelo	Agnus castus fruit	14194408	1
Caelo	Agnus castus fruit	13193410	2
Caelo	Agnus castus fruit	13193404	1
Caelo	Agnus castus fruit	1513546	1
Caelo	Agnus castus fruit	13193403	1
Caelo	Agnus castus fruit	13193401	2
Caelo	Agnus castus fruit	12274012	1
Caelo	Agnus castus fruit	12274013	2
Caelo	Agnus castus fruit	12274014	1
Caelo	Agnus castus fruit	80175158	2
Caelo	Agnus castus fruit	3413A-03015	1
Caelo	Agnus castus fruit	12016905	2
Caelo	Agnus castus fruit	12274009	2
Caelo	Agnus castus fruit	12274008	1
Caelo	Agnus castus fruit	12274002	1
Caelo	Agnus castus fruit	12274003	4
Caelo	Agnus castus fruit	12016902	1
Caelo	Agnus castus fruit	13193406	1
Caelo	Agnus castus fruit	12016909	4
Caelo	Agrimony, cut	10325502	2
Caelo	Agrimony, cut	11374005	2
Caelo	Agrimony, cut	11374006	6
Caelo	Agrimony, cut	3481-A-110324	1
Caelo	Agrimony, cut	10325505	1
Caelo	Agrimony, cut	12382903	1
Caelo	Agrimony, cut	12382901	3
Caelo	Agrimony, cut	1137407	1
Caelo	Alchemilla alpina her...	12147205	2
Caelo	Alchemilla alpina her...	1214204	1
Caelo	Alchemilla alpina her...	11063608	1
Caelo	Alchemilla alpina her...	12147206	3
Caelo	Alchemilla alpina her...	12147203-3470312131	1
Caelo	Alchemilla alpina her...	12147203	1
Caelo	Alchemilla alpina her...	12147202	3

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Supplier	Substance	Batch	Spectra
Caelo	Alchemilla, cut	13141101	7
Caelo	Alchemilla, cut	13141103	36
Caelo	Alchemilla, cut	1118206	1
Caelo	Alchemilla, cut	H-040513-2	1
Caelo	Alchemilla, cut	1213309	1
Caelo	Alchemilla, cut	125306	1
Caelo	Alchemilla, cut	14066003	1
Caelo	Alchemilla, cut	21081203	1
Caelo	Alchemilla, cut	11182807	2
Caelo	Alchemilla, cut	1406211616	1
Caelo	Alchemilla, cut	11182804	3
Caelo	Alchemilla, cut	11182801	3
Caelo	Alchemilla, cut	1215309	1
Caelo	Alchemilla, cut	5041301	1
Caelo	Alchemilla, cut	12342901	1
Caelo	Alchemilla, cut	27011401	1
Caelo	Alchemilla, cut	11182805	1
Caelo	Alchemilla, cut	12153306	5
Caelo	Alchemilla, cut	11063605	1
Caelo	Alchemilla, cut	1215305	2
Caelo	Alchemilla, cut	11182808	1
Caelo	Alchemilla, cut	12153301	3
Caelo	Alchemilla, cut	11002906	5
Caelo	Alchemilla, cut	8121201	1
Caelo	Alchemilla, cut	12153303	6
Caelo	Alchemilla, cut	15147002	2
Caelo	Alchemilla, cut	14066008	1
Caelo	Alchemilla, cut	13141106-3545412081	1
Caelo	Alchemilla, cut	12153305	25
Caelo	Alchemilla, cut	12153307	3
Caelo	Alchemilla, cut	1100912	1
Caelo	Alchemilla, cut	9011405	1
Caelo	Alchemilla, cut	2081304	1
Caelo	Alchemilla, cut	5013I1616	1
Caelo	Alchemilla, cut	13141106	8
Caelo	Alchemilla, cut	13141103-3456311103	1
Caelo	Alchemilla, cut	131411002	1
Caelo	Alchemilla, cut	13141105	3
Caelo	Alchemilla, cut	13141103-3400310161	1
Caelo	Alchemilla, cut	13141103-3382319003	1
Caelo	Alchemilla, cut	13091304	1
Caelo	Alchemilla, cut	13141102	6
Caelo	Alchemilla, cut	3613M01616	1
Caelo	Alchemilla, cut	intch:318080	1
Caelo	Alchemilla, cut	14066002	2
Caelo	Almonds, bitter, whole	16221202	1
Caelo	Almonds, bitter, whole	15193103	1
Caelo	Almonds, bitter, whole	5121301	1
Caelo	Almonds, bitter, whole	13242001	1
Caelo	Almonds, bitter, whole	12239604	1
Caelo	Aloes, cape, cut	25071402	1
Caelo	Aloes, cape, cut	12232102	1
Caelo	Aloes, cape, cut	12338201	4
Caelo	Aloes, cape, cut	12338203	4
Caelo	Aloes, cape, cut	505125	1
Caelo	Aloes, cape, cut	25111303	1
Caelo	Aloes, cape, cut	12338209	1
Caelo	Aloes, cape, cut	11041402	1
Caelo	Aloes, cape, cut	16202404	1
Caelo	Aloes, cape, cut	16202401	1

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Supplier	Substance	Batch	Spectra
Caelo	Aloes, cape, cut	15283001	1
Caelo	Aloes, cape, cut	11061406	1
Caelo	Aloes, cape, cut	12338206	2
Caelo	Aloes, cape, cut	15283010	1
Caelo	Aloes, cape, powdered	12183013	3
Caelo	Aloes, cape, powdered	11132116	1
Caelo	Aloes, cape, powdered	11132115	1
Caelo	Aloes, cape, powdered	12183007	1
Caelo	Aloes, cape, powdered	12183001	1
Caelo	Aloes, cape, powdered	12183009	3
Caelo	Aloes, cape, powdered	16202410	1
Caelo	Aloes, cape, powdered	15206514	1
Caelo	Aloes, cape, powdered	11132116	2
Caelo	Aloes, cape, powdered	15206516	1
Caelo	Aloes, cape, powdered	15206507	1
Caelo	Aloes, cape, powdered	14065905	1
Caelo	Aloes, cape, powdered	15206501	1
Caelo	Aloes, cape, powdered	14065906	1
Caelo	Aloes, cape, powdered	12183008	1
Caelo	Aluminium chloride he...	23111203	1
Caelo	Aluminium chloride he...	12114910	6
Caelo	Aluminium chloride he...	28121301	1
Caelo	Aluminium chloride he...	12323717	5
Caelo	Aluminium chloride he...	13L13-B03-287298	1
Caelo	Aluminium chloride he...	11229906	1
Caelo	Aluminium chloride he...	10251307	1
Caelo	Aluminium chloride he...	11229907	1
Caelo	Aluminium chloride he...	12114919	1
Caelo	Aluminium chloride he...	12114906	6
Caelo	Aluminium chloride he...	12114922	14
Caelo	Aluminium chloride he...	15080701	1
Caelo	Aluminium chloride he...	18061308	1
Caelo	Aluminium chloride he...	9071303	1
Caelo	Aluminium chloride he...	12323711	17
Caelo	Aluminium chloride he...	12114908	8
Caelo	Aluminium chloride he...	12047514	3
Caelo	Aluminium chloride he...	5081301	1
Caelo	Aluminium chloride he...	12114904	2
Caelo	Aluminium chloride he...	12047503	2
Caelo	Aluminium chloride he...	12114920	11
Caelo	Aluminium chloride he...	51/AD1	1
Caelo	Aluminium chloride he...	8031301	1
Caelo	Aluminium chloride he...	11229917	3
Caelo	Aluminium chloride he...	13G03-N02	21
Caelo	Aluminium chloride he...	15080715	1
Caelo	Aluminium chloride he...	13/13-B03-287298	1
Caelo	Aluminium chloride he...	12114918	17
Caelo	Aluminium chloride he...	12323710	8
Caelo	Aluminium chloride he...	11229914	1
Caelo	Aluminium chloride he...	15051302	1
Caelo	Aluminium chloride he...	3113E-01095	1
Caelo	Aluminium chloride he...	11229905	1
Caelo	Aluminium chloride he...	12021303	1
Caelo	Aluminium chloride he...		2
Caelo	Aluminium chloride he...	19041302	1
Caelo	Aluminium chloride he...	10251314	1
Caelo	Aluminium chloride he...	12127-N01	1
Caelo	Aluminium chloride he...	12114912	4
Caelo	Aluminium chloride he...	3091205	1
Caelo	Aluminium potassium s...	12184402	3

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Supplier	Substance	Batch	Spectra
Caelo	Aluminium potassium s...	12022409	1
Caelo	Aluminium potassium s...	15172501	1
Caelo	Aluminium potassium s...	12144602	1
Caelo	Aluminium potassium s...	12184407	3
Caelo	Aluminium potassium s...	12184411	1
Caelo	Aluminium potassium s...	12022444	1
Caelo	Aluminium potassium s...	12184406	2
Caelo	Aluminium potassium s...	12184408	3
Caelo	Aluminium potassium s...	12144607	2
Caelo	Aluminium potassium s...	12022406	1
Caelo	Aluminium potassium s...	12144605	4
Caelo	Aluminium potassium s...	90033229	1
Caelo	Aluminium potassium s...	12239102	2
Caelo	Aluminium potassium s...	12184401	1
Caelo	Aluminium potassium s...	1218411	1
Caelo	Aluminium potassium s...	504311092	1
Caelo	Aluminium potassium s...	13025401	3
Caelo	Aluminium potassium s...	2713Q1092	1
Caelo	Aluminium potassium s...	13025404	3
Caelo	Aluminium potassium s...	13098702	1
Caelo	Aluminium potassium s...	12 24-M03	1
Caelo	Aluminium potassium s...	12184401	1
Caelo	Aluminium potassium s...	12184407	5
Caelo	Aluminium potassium s...	14263804	1
Caelo	Aluminium potassium s...	12022406	2
Caelo	Aluminium potassium s...	12022401	1
Caelo	Aluminium potassium s...	11254805	1
Caelo	Aluminium potassium s...	11218611	2
Caelo	Aluminium potassium s...	12022404	1
Caelo	Aluminium potassium s...	510211092	1
Caelo	Aluminium potassium s...	11017211	1
Caelo	Aluminium potassium s...	12144603	1
Caelo	Ammonium chloride	12240302	4
Caelo	Ammonium chloride	10176309	1
Caelo	Ammonium chloride	10176319	2
Caelo	Ammonium chloride	12356101	3
Caelo	Ammonium hydrogen car...	3712Q-01103	1
Caelo	Ammonium hydrogen car...	23011404	1
Caelo	Ammonium hydrogen car...	3091204	1
Caelo	Ammonium hydrogen car...	72715338	1
Caelo	Ammonium hydrogen car...	12322204	1
Caelo	Ammonium hydrogen car...	24101202	1
Caelo	Ammonium hydrogen car...	25111308	1
Caelo	Ammonium hydrogen car...	9139402	1
Caelo	Ammonium hydrogen car...	13104601	1
Caelo	Ammonium hydrogen car...	11145612	2
Caelo	Ammonium hydrogen car...	12322201	1
Caelo	Ammonium hydrogen car...	12022308	2
Caelo	Ammonium hydrogen car...	13104611	1
Caelo	Amphetamine sulfate	15193204	1
Caelo	Amphetamine sulfate	12B06-N013	1
Caelo	Amphetamine sulfate	17K03-B01	1
Caelo	Amphetamine sulfate	15L01-B05	3
Caelo	Amphetamine sulfate	16153909	1
Caelo	Amphetamine sulfate	16153903	4
Caelo	Amphetamine sulfate	1807171	1
Caelo	Amphetamine sulfate	13344609	1
Caelo	Amphetamine sulfate	1ot067002	1
Caelo	Amphetamine sulfate	16153902	1
Caelo	Amphetamine sulfate	12I24-N03	1

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Supplier	Substance	Batch	Spectra
Caelo	Angelica root	12350703	9
Caelo	Angelica root	12168705	2
Caelo	Angelica root	10071306	1
Caelo	Angelica root	16128006	1
Caelo	Angelica root	6081B130109	7
Caelo	Angelica root	15101304	1
Caelo	Angelica root	5091303	1
Caelo	Angelica root	9030301	1
Caelo	Angelica root	12350705	1
Caelo	Angelica root	Int.Ch:318090	1
Caelo	Angelica root	30011302	1
Caelo	Angelica root	12350704	2
Caelo	Angelica root	13041711	1
Caelo	Angelica root	303299	1
Caelo	Angelica root	12168703	2
Caelo	Angelica root	12168701	3
Caelo	Angelica root	11093304	1
Caelo	Angelica root	16128002	1
Caelo	Angelica root	5162606	1
Caelo	Angelica root	15162604	2
Caelo	Angelica root	14179506	2
Caelo	Angelica root	14178506	1
Caelo	Angelica root	28101402	1
Caelo	Angelica root	12080412	1
Caelo	Angelica root	285732	2
Caelo	Angelica root	12080403	1
Caelo	Angelica root	21011402	1
Caelo	Angelica root	269740	1
Caelo	Angelica root	17053301	1
Caelo	Aniseed	15046101	5
Caelo	Aniseed	15283201	3
Caelo	Aniseed	15046106	1
Caelo	Aniseed	15398603	3
Caelo	Aniseed	13037807	1
Caelo	Aniseed	2215M-01530	1
Caelo	Aniseed	13333914	1
Caelo	Aniseed	15049103	1
Caelo	Aniseed	15046102	8
Caelo	Aniseed	13333916	1
Caelo	Aniseed	15398605	5
Caelo	Aniseed	15046110	1
Caelo	Aniseed	16165303	1
Caelo	Aniseed	15398607	1
Caelo	Aniseed	16165305	5
Caelo	Aniseed	2916E-01530	1
Caelo	Aniseed	15398602	5
Caelo	Aniseed	16165302	1
Caelo	Aniseed	16165304	3
Caelo	Aniseed	15046109	5
Caelo	Aniseed	15046103	3
Caelo	Aniseed	16165308	1
Caelo	Aniseed	11101203	6
Caelo	Aniseed	13037805	11
Caelo	Aniseed	5091304	1
Caelo	Aniseed	13333910	4
Caelo	Aniseed	13037901	1
Caelo	Aniseed	140913a	1
Caelo	Aniseed	13037803	2
Caelo	Aniseed	PrüfNr4913E-01530	1
Caelo	Aniseed	13333912	3

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Supplier	Substance	Batch	Spectra
Caelo	Aniseed	13333909	2
Caelo	Aniseed	13037801	1
Caelo	Aniseed	13333906	3
Caelo	Aniseed	13333907	4
Caelo	Aniseed	13333908	7
Caelo	Aniseed	13333902	9
Caelo	Aniseed		1
Caelo	Aniseed	13333903	3
Caelo	Aniseed	12360801	1
Caelo	Aniseed	13037808-3560412014	1
Caelo	Aniseed	13333901	6
Caelo	Aniseed	13037809	12
Caelo	Aniseed	5121401	1
Caelo	Aniseed	13037804	7
Caelo	Aniseed	5061301	1
Caelo	Aniseed	4061301	1
Caelo	Aniseed	111101213	1
Caelo	Aniseed	11101202	3
Caelo	Aniseed	11101213	2
Caelo	Aniseed	10081207	1
Caelo	Aniseed	11101201	1
Caelo	Aniseed	11101215	3
Caelo	Aniseed	11370301	10
Caelo	Aniseed	17045603	1
Caelo	Aniseed	12226402	5
Caelo	Aniseed	11101214	6
Caelo	Aniseed	11370303	11
Caelo	Aniseed	10247202	1
Caelo	Aniseed	17045601	1
Caelo	Aniseed	17045611	1
Caelo	Aniseed	17045609	1
Caelo	Aniseed	11121705	1
Caelo	Aniseed	1137033	1
Caelo	Aniseed	11370302	4
Caelo	Aniseed	11370308	3
Caelo	Aniseed	13037802	9
Caelo	Aniseed	3314E-01530	1
Caelo	Aniseed	16165306	2
Caelo	Aniseed	13037808	9
Caelo	Aniseed, pounded	13149902	1
Caelo	Aniseed, pounded	12111303	3
Caelo	Aniseed, pounded	11242003	1
Caelo	Aniseed, pounded	12360803	2
Caelo	Aniseed, pounded	4041302	1
Caelo	Aniseed, pounded	23041303	1
Caelo	Aniseed, pounded	12111304	1
Caelo	Aniseed, pounded	15149702	1
Caelo	Aniseed, pounded	1314990	1
Caelo	Apple, cut	12227301	1
Caelo	Arnica flower	11374103	1
Caelo	Arnica flower	1222702	1
Caelo	Arnica flower	12227203	1
Caelo	Arnica flower	6112013A	1
Caelo	Arnica flower	11285703	1
Caelo	Arnica flower	11374102	2
Caelo	Arnica flower	11259803	1
Caelo	Arnica flower	IntCh:212032	1
Caelo	Arnica flower	12227202	1
Caelo	Arnica flower	11374105	1
Caelo	Arnica flower	11374101	2

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Supplier	Substance	Batch	Spectra
Caelo	Arnica flower	10207405	1
Caelo	Arnica flower	28071201	1
Caelo	Arnica flower	11259804	1
Caelo	Arnica flower	10081204	1
Caelo	Arnica flower	11285705	1
Caelo	Arnica flower	12227202	1
Caelo	Artichoke leaf, cut	12173302	3
Caelo	Artichoke leaf, cut	12173304	2
Caelo	Artichoke leaf, cut	13037608	1
Caelo	Artichoke leaf, cut	13037607	4
Caelo	Artichoke leaf, cut	81232298	1
Caelo	Artichoke leaf, cut	12173307-3260315072	1
Caelo	Artichoke leaf, cut	13310706	1
Caelo	Artichoke leaf, cut	13037603	1
Caelo	Artichoke leaf, cut	2312I-03593	1
Caelo	Artichoke leaf, cut	12173307	6
Caelo	Artichoke leaf, cut	12173306	2
Caelo	Ash leaf, cut	12225504	1
Caelo	Ash leaf, cut	12225505	2
Caelo	Ash leaf, cut	12225502	1
Caelo	Asparagus root, cut	13193302	1
Caelo	Barberries	12217116	1
Caelo	Barberries	16224202	1
Caelo	Barberries	12217113	2
Caelo	Barberries	12217111	1
Caelo	Barberries	12217106	1
Caelo	Barberries	12217109	4
Caelo	Barberries	11058320	1
Caelo	Barberries	12217103	3
Caelo	Barberries	12217107	1
Caelo	Barberries	1221707	1
Caelo	Barberry root bark, cut	12112608	1
Caelo	Barberry root bark, cut	12112606	4
Caelo	Barberry root bark, cut	12112605	1
Caelo	Barberry root bark, cut	11083509	1
Caelo	Barberry root bark, cut	55B110128	1
Caelo	Barberry root bark, cut	12112603	2
Caelo	Basil, rubbed	12007008	2
Caelo	Basil, rubbed	12007010	3
Caelo	Basil, rubbed	12066404	1
Caelo	Basil, rubbed	13048605-3519411022	1
Caelo	Basil, rubbed	13048605	1
Caelo	Basil, rubbed	13048601	2
Caelo	Bean shells, cut	10006507	1
Caelo	Bean shells, cut	8301004	1
Caelo	Bean shells, cut	11030602	5
Caelo	Bean shells, cut	11233603	1
Caelo	Bean shells, cut	15060905	1
Caelo	Bean shells, cut	6031301	1
Caelo	Bean shells, cut	29091201	1
Caelo	Bean shells, cut	14080002	1
Caelo	Bean shells, cut	13333803	1
Caelo	Bean shells, cut	1333802	1
Caelo	Bean shells, cut	13333801	1
Caelo	Bean shells, cut	1103061	1
Caelo	Bean shells, cut	12358703	5
Caelo	Bean shells, cut	11030601	1
Caelo	Bean shells, cut	11030605	1
Caelo	Bean shells, cut	11030604	5
Caelo	Bearberry leaf, cut	11213011	3

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Supplier	Substance	Batch	Spectra
Caelo	Bearberry leaf, cut	20111210	1
Caelo	Bearberry leaf, cut	1218602	1
Caelo	Bearberry leaf, cut	11213010	1
Caelo	Bearberry leaf, cut	12186502	1
Caelo	Bearberry leaf, cut	12186506	3
Caelo	Bearberry leaf, cut	12186503	1
Caelo	Bearberry leaf, cut	15051303	1
Caelo	Bearberry leaf, cut	4091301	1
Caelo	Bearberry leaf, cut	13067805	6
Caelo	Bearberry leaf, cut	5111301	1
Caelo	Bearberry leaf, cut	12186504	1
Caelo	Bearberry leaf, cut	11213005	4
Caelo	Bearberry leaf, cut	17121306	1
Caelo	Bearberry leaf, cut	280889	3
Caelo	Bearberry leaf, cut	4021407	1
Caelo	Bearberry leaf, cut	412A-01518	1
Caelo	Bearberry leaf, cut	13067802	2
Caelo	Bearberry leaf, cut	15116201	1
Caelo	Bearberry leaf, cut	13067805-3390311080	1
Caelo	Bentonite	1307016-01	1
Caelo	Bentonite	fürHerrSalloch	1
Caelo	Bentonite	1311014-01	1
Caelo	Betamethasone-17-vale. ...	12A05-N08	3
Caelo	Betamethasone-17-vale. ...	12a05-no8	1
Caelo	Betony herb, cut	13367802	1
Caelo	Betony herb, cut	13048906	1
Caelo	Betony herb, cut	12007208	1
Caelo	Betony herb, cut	12007201	1
Caelo	Betony herb, cut	134048903	1
Caelo	Bilberry fruit, dried	13130504	1
Caelo	Bilberry fruit, dried	10273709	1
Caelo	Bilberry fruit, dried	10273711	1
Caelo	Bilberry fruit, dried	12183701	2
Caelo	Bilberry fruit, dried	26061301	1
Caelo	Bilberry fruit, dried	12183704	4
Caelo	Bilberry fruit, dried	13130501	1
Caelo	Bilberry fruit, dried	10273708	1
Caelo	Bilberry fruit, dried	18101307	1
Caelo	Bilberry fruit, dried	10265603	1
Caelo	Bilberry fruit, dried	10265601	1
Caelo	Bilberry leaf, cut	1300907	1
Caelo	Bilberry leaf, cut	13009907	2
Caelo	Bilberry leaf, cut	3091302	1
Caelo	Bilberry leaf, cut	12140206	2
Caelo	Bilberry leaf, cut	13009901	3
Caelo	Bilberry leaf, cut	13009903	4
Caelo	Bilberry leaf, cut	23111201	1
Caelo	Bilberry leaf, cut	9367603	2
Caelo	Bilberry leaf, cut	12140204	4
Caelo	Bilberry leaf, cut	12140201	2
Caelo	Bilberry leaf, cut	13009904	3
Caelo	Birch leaf, cut	IntCh:311092	1
Caelo	Birch leaf, cut	14360702	1
Caelo	Birch leaf, cut	11189502	1
Caelo	Birch leaf, cut	12193108	1
Caelo	Birch leaf, cut	11189507	1
Caelo	Birch leaf, cut	11189510	3
Caelo	Birch leaf, cut	13337303-3561412013	1
Caelo	Birch leaf, cut	13108905	8
Caelo	Birch leaf, cut	12193105	3

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Supplier	Substance	Batch	Spectra
Caelo	Birch leaf, cut	13337303	1
Caelo	Birch leaf, cut	107063	1
Caelo	Birch leaf, cut	12193004	5
Caelo	Birch leaf, cut	12193104	1
Caelo	Birch leaf, cut	11189508	1
Caelo	Birch leaf, cut	13337302	1
Caelo	Birch leaf, cut	13108917	1
Caelo	Birch leaf, cut	12193109	15
Caelo	Birch leaf, cut	13108916	1
Caelo	Birch leaf, cut	13108906	1
Caelo	Bitter fennel	15141004	1
Caelo	Bitter fennel	15006507	1
Caelo	Bitter fennel	14376406	1
Caelo	Bitter fennel	15006508	2
Caelo	Bitter fennel	5061302	1
Caelo	Bitter fennel	15006501	1
Caelo	Bitter fennel	14376408;21S08	1
Caelo	Bitter fennel	4061302	1
Caelo	Bitter fennel	154443204	1
Caelo	Bitter fennel	12094716	6
Caelo	Bitter fennel	15006506	1
Caelo	Bitter fennel	15443203	2
Caelo	Bitter fennel	16005902	1
Caelo	Bitter fennel	15443205	2
Caelo	Bitter fennel	15443206	1
Caelo	Bitter fennel	15443204	6
Caelo	Bitter fennel	15443208	1
Caelo	Bitter fennel	12094712	4
Caelo	Bitter fennel	15443202	3
Caelo	Bitter fennel	15443212	3
Caelo	Bitter fennel	15443209	2
Caelo	Bitter fennel	14376401	1
Caelo	Bitter fennel	15443215	1
Caelo	Bitter fennel	15007601	1
Caelo	Bitter fennel	13148305	2
Caelo	Bitter fennel	12167101	1
Caelo	Bitter fennel	12362710	1
Caelo	Bitter fennel	13148303	2
Caelo	Bitter fennel	14111301	1
Caelo	Bitter fennel	13148304	18
Caelo	Bitter fennel	12094726	2
Caelo	Bitter fennel	13200401	4
Caelo	Bitter fennel	9121305	1
Caelo	Bitter fennel	12094716-3408310191	1
Caelo	Bitter fennel	13020802	6
Caelo	Bitter fennel	1250117/15443216	1
Caelo	Bitter fennel	12094721	3
Caelo	Bitter fennel	12094719	4
Caelo	Bitter fennel	12094725	5
Caelo	Bitter fennel	12094724	3
Caelo	Bitter fennel	1302081	1
Caelo	Bitter fennel	7031306	1
Caelo	Bitter fennel	13200402	2
Caelo	Bitter fennel	1320041	1
Caelo	Bitter fennel	13020801	4
Caelo	Bitter fennel	12345678	1
Caelo	Bitter fennel	14376402	1
Caelo	Bitter fennel	14376405	1
Caelo	Bitter fennel	13398502	1
Caelo	Bitter fennel	14255802	3

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Supplier	Substance	Batch	Spectra
Caelo	Bitter fennel	13148304-3500411070	1
Caelo	Bitter fennel	5121401	1
Caelo	Bitter fennel	13371610	2
Caelo	Bitter fennel	12094715	4
Caelo	Bitter fennel	13371610	1
Caelo	Bitter fennel	13371605	1
Caelo	Bitter fennel	13148306	1
Caelo	Bitter fennel	13148307	1
Caelo	Bitter fennel	13398502	1
Caelo	Bitter fennel	2150317	1
Caelo	Bitter fennel	16061202	1
Caelo	Bitter fennel	12094710	4
Caelo	Bitter fennel	11185501	1
Caelo	Bitter fennel	12094717	1
Caelo	Bitter fennel	16298102	1
Caelo	Bitter fennel	12035102	1
Caelo	Bitter fennel	6091201	1
Caelo	Bitter fennel	12094705	3
Caelo	Bitter fennel	12094703	2
Caelo	Bitter fennel	1209474	1
Caelo	Bitter fennel	12035102	2
Caelo	Bitter fennel	12094720	5
Caelo	Bitter fennel	12094704	3
Caelo	Bitter fennel	402311545	1
Caelo	Bitter fennel	12094707	4
Caelo	Bitter fennel	11016330	1
Caelo	Bitter fennel	12167102	4
Caelo	Bitter fennel	27121201	1
Caelo	Bitter orange flower ...	13352701-3518411022	1
Caelo	Bitter orange flower ...	13352701	1
Caelo	Bitter orange flower ...	13067903	2
Caelo	Bitter orange flower ...	12266708	1
Caelo	Bitter orange flower ...	12266611	1
Caelo	Bitter orange flower ...	12266608	2
Caelo	Bitter orange flower ...	6051301	1
Caelo	Bitter orange flower ...	12266609	1
Caelo	Bitter orange flower ...	2712E-01445	1
Caelo	Bitter orange flower ...	12266608	6
Caelo	Bitter orange flower ...	12266605	1
Caelo	Bitter orange flower ...	11049202	1
Caelo	Bitter orange flower ...	12266703	2
Caelo	Bitter orange flower ...	11049212	1
Caelo	Bitter orange flower ...	12266605	1
Caelo	Bitter orange flower ...	12266707	1
Caelo	Bitter orange flower ...	12266614	1
Caelo	Bitter orange flower ...	12266705	1
Caelo	Bitter orange flower ...	12266611	1
Caelo	Bitter orange peel, cut	27011403	1
Caelo	Bitter orange peel, cut	21101302	1
Caelo	Bitter orange peel, cut	13049001	1
Caelo	Bitter orange peel, cut	4312M-01531	1
Caelo	Bitter orange peel, cut	12239203	3
Caelo	Bitter orange peel, cut	17111201	1
Caelo	Bitter orange peel, cut	12067402	1
Caelo	Bitter orange peel, cut	12067405	1
Caelo	Black cohosh, cut	10281112	1
Caelo	Black cohosh, cut	10281104	1
Caelo	Black cohosh, cut	10281118	2
Caelo	Black cohosh, cut	13142101	1
Caelo	Black cohosh, cut	13237901	2

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Supplier	Substance	Batch	Spectra
Caelo	Black cohosh, cut	13237903	1
Caelo	Black cumin seed	12358904	1
Caelo	Black cumin seed	12358901	2
Caelo	Black cumin seed	10121916	1
Caelo	Black cumin seed	14359903	3
Caelo	Black cumin seed	14359905	1
Caelo	Black cumin seed	12358902	1
Caelo	Black cumin seed	12358903	2
Caelo	Black cumin seed	11233502	2
Caelo	Black cumin seed	11233503	1
Caelo	Black cumin seed	13326406	1
Caelo	Black cumin seed	11233507	1
Caelo	Black cumin seed	15300401	1
Caelo	Black cumin seed	16115703	1
Caelo	Black cumin seed	13326405	2
Caelo	Black cumin seed	12358906	2
Caelo	Black cumin seed	16115708	1
Caelo	Black cumin seed	13122013b	1
Caelo	Black cumin seed	10121915	1
Caelo	Black mustard seed	13038904	1
Caelo	Black mustard seed	14057702	1
Caelo	Black mustard seed	12189307	1
Caelo	Black mustard seed, p...	17276404	1
Caelo	Black mustard seed, p...	12350211	3
Caelo	Black mustard seed, p...	16051802	2
Caelo	Black mustard seed, p...	17196306	1
Caelo	Black mustard seed, p...	14162810	2
Caelo	Black mustard seed, p...	12009706	1
Caelo	Black mustard seed, p...	12009703	1
Caelo	Black mustard seed, p...	12009702	4
Caelo	Black mustard seed, p...	14162810	3
Caelo	Black mustard seed, p...	11276701	1
Caelo	Black mustard seed, p...	12208602	5
Caelo	Black mustard seed, p...	14162807	2
Caelo	Black mustard seed, p...	14293701	2
Caelo	Black mustard seed, p...	14293702	6
Caelo	Black mustard seed, p...	14162802	1
Caelo	Black mustard seed, p...	14162808	1
Caelo	Black mustard seed, p...	17196303	3
Caelo	Black mustard seed, p...	14293706	1
Caelo	Black mustard seed, p...	14245601	1
Caelo	Black mustard seed, p...	23061401	1
Caelo	Black mustard seed, p...	12208604	3
Caelo	Black mustard seed, p...	12208601	3
Caelo	Black mustard seed, p...	13097706	2
Caelo	Black mustard seed, p...	13097702	4
Caelo	Black mustard seed, p...	13097705	6
Caelo	Black mustard seed, p...	12350209	1
Caelo	Black mustard seed, p...	13097704	4
Caelo	Black mustard seed, p...	12350202-3369319012	1
Caelo	Black mustard seed, p...	13358302	13
Caelo	Black mustard seed, p...	25011401	1
Caelo	Black mustard seed, p...	13097701	11
Caelo	Black mustard seed, p...	12350207	5
Caelo	Black mustard seed, p...	13358304	4
Caelo	Black mustard seed, p...	12350204	2
Caelo	Black mustard seed, p...	12350208	7
Caelo	Black mustard seed, p...	12350205	2
Caelo	Black mustard seed, p...	12350202	16
Caelo	Black mustard seed, p...	14293713	1

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Supplier	Substance	Batch	Spectra
Caelo	Black mustard seed, p...	2015Q-02244	1
Caelo	Black mustard seed, p...	14293710	2
Caelo	Black mustard seed, p...	15131102	3
Caelo	Black mustard seed, p...	1633503	1
Caelo	Black mustard seed, p...	16333503	2
Caelo	Black mustard seed, p...	16333501	1
Caelo	Black mustard seed, p...	16272707	3
Caelo	Black mustard seed, p...	16272704	1
Caelo	Black mustard seed, p...	16272703	6
Caelo	Black mustard seed, p...	16051810	3
Caelo	Black mustard seed, p...	16051807	1
Caelo	Black mustard seed, p...	16051807	1
Caelo	Black mustard seed, p...	15131104	1
Caelo	Black mustard seed, p...	15214714	1
Caelo	Black mustard seed, p...	12350210	1
Caelo	Black mustard seed, p...	15214707	1
Caelo	Black mustard seed, p...	15131105	1
Caelo	Black mustard seed, p...	15131101	1
Caelo	Black mustard seed, p...	15214703	4
Caelo	Black mustard seed, p...	15214706	3
Caelo	Black mustard seed, p...	15214703	1
Caelo	Black mustard seed, p...	15214708	3
Caelo	Black mustard seed, p...	15214713	2
Caelo	Black pepper	12192306	1
Caelo	Black pepper	13221110	1
Caelo	Black pepper	12192309	1
Caelo	Black pepper	15395310	1
Caelo	Black pepper	11193911	1
Caelo	Black pepper	12192305	1
Caelo	Black pepper	12192304	1
Caelo	Blackberry leaf, cut	10136403	1
Caelo	Blackberry leaf, cut	10136408	6
Caelo	Blackberry leaf, cut	28061202	1
Caelo	Blackberry leaf, cut	13091206	1
Caelo	Blackberry leaf, cut	11030701	2
Caelo	Blackberry leaf, cut	11030706	1
Caelo	Blackberry leaf, cut	2271c120508	1
Caelo	Blackberry leaf, cut	11030707	5
Caelo	Blackberry leaf, cut	15039301	1
Caelo	Blackberry leaf, cut	14019010	1
Caelo	Blackberry leaf, cut	13101610	1
Caelo	Blackberry leaf, cut	13127901	1
Caelo	Blackberry leaf, cut	3011E-01512	1
Caelo	Blackberry leaf, cut	11030704	3
Caelo	Blackberry leaf, cut	14111318	1
Caelo	Blackberry leaf, cut	3091303	1
Caelo	Blackcurrant leaf, cut	80558228	1
Caelo	Blackcurrant leaf, cut	12168804	1
Caelo	Blackcurrant leaf, cut	12168810	3
Caelo	Blackcurrant leaf, cut	9373913	1
Caelo	Blackcurrant leaf, cut	12115902	1
Caelo	Blackcurrants	12272804	3
Caelo	Blackthorn flower	12178103	2
Caelo	Blackthorn flower	12178102	9
Caelo	Blackthorn flower	11206906	1
Caelo	Blackthorn flower	12178104	4
Caelo	Blackthorn flower	12178105	1
Caelo	Blackthorn flower	12178101	1
Caelo	Blackthorn flower, ru...	1150N101109	2
Caelo	Blessed thistle, cut	13025902	1

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Supplier	Substance	Batch	Spectra
Caelo	Blessed thistle, cut	13389701	1
Caelo	Blessed thistle, cut	13025903	3
Caelo	Blessed thistle, cut	3091301	1
Caelo	Blessed thistle, cut	12038202	1
Caelo	Blessed thistle, cut	4743554	1
Caelo	Blessed thistle, cut	10325404	1
Caelo	Blessed thistle, cut	10325402	5
Caelo	Blessed thistle, cut	27111205	1
Caelo	Blessed thistle, cut	12038203	2
Caelo	Blessed thistle, cut	9355208	1
Caelo	Blessed thistle, cut	13025901	5
Caelo	Blue bottle flower wi...	12060202	2
Caelo	Blue bottle flower wi...	11059209	2
Caelo	Blue bottle flower wi...	12232501	2
Caelo	Blue bottle flower wi...	12060203	4
Caelo	Blue bottle flower wi...	11059206	2
Caelo	Blue bottle flower wi...	11059211	2
Caelo	Blue bottle flower wi...	14323302	1
Caelo	Blue bottle flower wi...	12060205	4
Caelo	Blue bottle flower wi...	15206601	1
Caelo	Bogbean leaf, cut	13149001	1
Caelo	Bogbean leaf, cut	13123902	2
Caelo	Bogbean leaf, cut	13123901	2
Caelo	Bogbean leaf, cut	12226104	1
Caelo	Bogbean leaf, cut	1226101	1
Caelo	Bogbean leaf, cut	12226101	1
Caelo	Boldo leaf, cut	12064305	1
Caelo	Boldo leaf, cut	11016509	1
Caelo	Boldo leaf, cut	11016511	1
Caelo	Boldo leaf, cut	655456	1
Caelo	Boldo leaf, cut	12227005	1
Caelo	Boldo leaf, cut	12064306	1
Caelo	Boldo leaf, cut	12227004	1
Caelo	Boldo leaf, cut	12064303	1
Caelo	Bucho leaf	13056605	1
Caelo	Bucho leaf	13056602	2
Caelo	Bucho leaf	13056601	2
Caelo	Buckwheat herb, cut	11212814	2
Caelo	Buckwheat herb, cut	11212809	1
Caelo	Buckwheat herb, cut	13051303	1
Caelo	Buckwheat herb, cut	30041301	1
Caelo	Buckwheat herb, cut	11212810	1
Caelo	Buckwheat herb, cut	11212808	2
Caelo	Buckwheat herb, cut	11212812	1
Caelo	Buckwheat herb, cut	13193203	1
Caelo	Buckwheat herb, cut	11212807	2
Caelo	Buckwheat herb, cut	5111302	1
Caelo	Buckwheat herb, cut	2051303	1
Caelo	Buckwheat herb, cut	11212612	1
Caelo	Buckwheat herb, cut	11212817	6
Caelo	Burdock root, cut	13122802	1
Caelo	Burdock root, cut	13122801	2
Caelo	Burdock root, cut	12295805	2
Caelo	Burdock root, cut	12295807	1
Caelo	Burdock root, cut	12295808	2
Caelo	Burdock root, cut	107063	1
Caelo	Burdock root, cut	12295802	3
Caelo	Burdock root, cut	11100801	2
Caelo	Burdock root, cut	10073213	1
Caelo	Burdock root, cut	1100801	1

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Supplier	Substance	Batch	Spectra
Caelo	Burdock root, cut	12295801	2
Caelo	Burnet root	12027411	3
Caelo	Burnet root	12027405	2
Caelo	Burnet root	12027413	1
Caelo	Burnet root	12027410	3
Caelo	Burnet root	8111203	1
Caelo	Burnet root	12027403	1
Caelo	Burnet root	12027409	1
Caelo	Caffeine citrate	13D30-N02	9
Caelo	Caffeine citrate	11F21-N05	1
Caelo	Calcium chloride dihy...	12341409	1
Caelo	Calcium chloride dihy...	12B09-N11	1
Caelo	Calcium chloride dihy...	12341404	2
Caelo	Calcium chloride dihy...	11230915	1
Caelo	Calcium chloride dihy...	11230921	2
Caelo	Calcium chloride dihy...	8237314	1
Caelo	Calcium chloride dihy...	12341406	1
Caelo	Calcium hydrogen phos...	14085301	1
Caelo	Calcium hydrogen phos...	101352009	1
Caelo	Calcium hydrogen phos...	10135216	1
Caelo	Calcium hydrogen phos...	12212806	1
Caelo	Calcium hydrogen phos...	12212804	5
Caelo	Calcium hydrogen phos...	11287509	2
Caelo	Calcium hydrogen phos...	12212813	1
Caelo	Calcium hydrogen phos...	12212807	1
Caelo	Calcium hydrogen phos...	11287501	1
Caelo	Calcium hydrogen phos...	10135223	1
Caelo	Calcium hydrogen phos...	12212812	2
Caelo	Calcium hydrogen phos...	10135228	1
Caelo	Calcium hydrogen phos...	13170704	2
Caelo	Calcium hydrogen phos...	12212816	1
Caelo	Calcium hydrogen phos...	13170701	5
Caelo	Calcium hydrogen phos...	14011401	1
Caelo	Calcium hydrogen phos...	11287503	2
Caelo	Calcium hydrogen phos...	12212822	1
Caelo	Calcium hydrogen phos...	12212811	5
Caelo	Calcium hydrogen phos...	11287510	1
Caelo	Calcium hydrogen phos...	10135201	1
Caelo	Calcium sulfate dihyd...	10132403	1
Caelo	Calcium sulfate dihyd...	12316301	1
Caelo	Calendula flower	13235502	3
Caelo	Calendula flower	13235503	3
Caelo	Calendula flower	12221510-3435311151	1
Caelo	Calendula flower	12221511	1
Caelo	Calendula flower	12221710	1
Caelo	Calendula flower	12221508	1
Caelo	Calendula flower	15291501	1
Caelo	Calendula flower	12221705	1
Caelo	Calendula flower	12221510-3356319071	1
Caelo	Calendula flower	12221708	3
Caelo	Calendula flower	12221706	2
Caelo	Calendula flower	122221707	1
Caelo	Calendula flower, cut	22061203	1
Caelo	Calendula flower, cut	18121301	1
Caelo	Calendula flower, cut	12221502	2
Caelo	Calendula flower, cut	11221407	1
Caelo	Calendula flower, cut	122221704	1
Caelo	Calendula flower, cut	21091301	1
Caelo	Calendula flower, cut	AKD1	1
Caelo	Calendula flower, cut	12221710	2

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Supplier	Substance	Batch	Spectra
Caelo	Calendula flower, cut	13235502	9
Caelo	Calendula flower, cut	9112013C	1
Caelo	Calendula flower, cut	13235501	4
Caelo	Calendula flower, cut	9121303	1
Caelo	Calendula flower, cut	12221705	4
Caelo	Calendula flower, cut	13235506	2
Caelo	Calendula flower, cut	10291904	1
Caelo	Calendula flower, cut	1325502	1
Caelo	Calendula flower, cut	19111206	1
Caelo	Calendula flower, cut	31121202	1
Caelo	Calendula flower, cut	11187611	3
Caelo	Calendula flower, cut	13235505	1
Caelo	Calendula flower, cut	3061301	1
Caelo	Calendula flower, cut	5021305	1
Caelo	Calendula flower, cut	12221707	2
Caelo	Calendula flower, cut	8041302	1
Caelo	Calendula flower, cut	295556	1
Caelo	Calendula flower, cut	12221701	1
Caelo	Calendula flower, cut	15040301	1
Caelo	Calendula flower, cut	11187610	3
Caelo	Calendula flower, cut	1187612	2
Caelo	Calendula flower, cut	12221704	11
Caelo	Calendula flower, cut	11187612	11
Caelo	Calendula flower, cut	12071201	1
Caelo	Calendula flower, cut	12221708	11
Caelo	Calendula flower, cut	13410202	2
Caelo	Calendula flower, cut	27101201	1
Caelo	Caraway fruit	15097109	1
Caelo	Caraway fruit	15097103	3
Caelo	Caraway fruit	15409103	1
Caelo	Caraway fruit	290416	1
Caelo	Caraway fruit	15097115	6
Caelo	Caraway fruit	15097116	1
Caelo	Caraway fruit	16308501	1
Caelo	Caraway fruit	15409105	1
Caelo	Caraway fruit	15409104	2
Caelo	Caraway fruit	2041017/16308501	1
Caelo	Caraway fruit	11121704	1
Caelo	Caraway fruit	18121717	1
Caelo	Caraway fruit	17256303	1
Caelo	Caraway fruit	15097111	1
Caelo	Caraway fruit	15097107	2
Caelo	Caraway fruit	4061303	1
Caelo	Caraway fruit	1509101	1
Caelo	Caraway fruit	12226608	3
Caelo	Caraway fruit	12226504	1
Caelo	Caraway fruit	12226606	2
Caelo	Caraway fruit	11378309	1
Caelo	Caraway fruit	12226604	4
Caelo	Caraway fruit	12226601	1
Caelo	Caraway fruit	9267815	1
Caelo	Caraway fruit	2103311537	1
Caelo	Caraway fruit	11003211	1
Caelo	Caraway fruit	12343403	1
Caelo	Caraway fruit	27121202	1
Caelo	Caraway fruit	12226501	5
Caelo	Caraway fruit	11003217	5
Caelo	Caraway fruit	811E-01537	1
Caelo	Caraway fruit	11003207	1
Caelo	Caraway fruit	413M	1

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Supplier	Substance	Batch	Spectra
Caelo	Caraway fruit	12226609	5
Caelo	Caraway fruit	12226614	2
Caelo	Caraway fruit	12226611	3
Caelo	Caraway fruit	15097101	8
Caelo	Caraway fruit	13306008	1
Caelo	Caraway fruit	13306006	4
Caelo	Caraway fruit	13306005	2
Caelo	Caraway fruit	13306004	1
Caelo	Caraway fruit	13397105	8
Caelo	Caraway fruit	13091401	1
Caelo	Caraway fruit	15097108	3
Caelo	Caraway fruit	13397104	2
Caelo	Caraway fruit	13306003	1
Caelo	Caraway fruit	13041901	1
Caelo	Caraway fruit	13041903	1
Caelo	Caraway fruit	13306002	5
Caelo	Caraway fruit	1222608	1
Caelo	Caraway fruit	1226608	1
Caelo	Caraway fruit	12226612	8
Caelo	Caraway fruit	13397102	2
Caelo	Caraway fruit	12226603	7
Caelo	Caraway fruit, pounded	12116904	3
Caelo	Caraway fruit, pounded	13367101	1
Caelo	Cardamom fruit	11309110	1
Caelo	Cardamom fruit	13026003	1
Caelo	Cardamom fruit	13260502-3537411072	1
Caelo	Cayenne pepper, powde...	13205106	1
Caelo	Celery root, cut	12319105	2
Caelo	Celery root, cut	12319107	1
Caelo	Celery root, cut	10270012	1
Caelo	Celery root, cut	10270009	1
Caelo	Celery root, cut	12319108	1
Caelo	Centaury, cut	12268602	16
Caelo	Centaury, cut	15224102	1
Caelo	Centaury, cut	3711B120628	1
Caelo	Centaury, cut	12268608	10
Caelo	Centaury, cut	12379601	1
Caelo	Centaury, cut	12268605	4
Caelo	Centaury, cut	12268601	3
Caelo	Centaury, cut	12268606	13
Caelo	Centaury, cut	11097602	1
Caelo	Centaury, cut	8021302	1
Caelo	Centaury, cut	11097605	2
Caelo	Centaury, cut	11097609	3
Caelo	Centaury, cut	10104012	1
Caelo	Ceylonese Cinnamon, p...	12242806	2
Caelo	Ceylonese Cinnamon, p...	12242818	1
Caelo	Ceylonese Cinnamon, p...	12242815	1
Caelo	Chelidonium majus her...	311092	1
Caelo	Chickweed, cut	13040503	1
Caelo	Chickweed, cut	13040504	1
Caelo	Chickweed, cut	13040501	1
Caelo	Chickweed, cut	13254401	1
Caelo	Chickweed, cut	13254403	2
Caelo	Chickweed, cut	4551B130902	1
Caelo	Chickweed, cut	13254404	1
Caelo	Chickweed, cut	13040502-3283310662	1
Caelo	Chickweed, cut	13040502	2
Caelo	Chickweed, cut	14212411	1
Caelo	Chicory herb, cut	14031315	1

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Supplier	Substance	Batch	Spectra
Caelo	Chicory herb, cut	12354302	3
Caelo	Chicory herb, cut	12354306	1
Caelo	Chicory herb, cut	12034303	3
Caelo	Chicory herb, cut	12034302	1
Caelo	Chicory herb, cut	12034301	2
Caelo	Chicory herb, cut	12369102	3
Caelo	Chicory root, cut	11374510	2
Caelo	Chicory root, cut	6221A101202	4
Caelo	Chicory root, cut	11081803	1
Caelo	Chicory root, cut	11374504	3
Caelo	Chicory root, cut	11374506	1
Caelo	Chicory root, cut	91338319	1
Caelo	Chicory root, cut	6221As101202	1
Caelo	Cinchona bark, cut	15301904	2
Caelo	Cinchona bark, cut	14009305	1
Caelo	Cinchona bark, cut	10381906	1
Caelo	Cinnamon rods (Ceylon...	12148904	1
Caelo	Cinnamon, cut	15151905	1
Caelo	Cinnamon, cut	13304409	1
Caelo	Cinnamon, cut	15151902	1
Caelo	Cinnamon, cut	16061702	1
Caelo	Cinnamon, cut	13304415	1
Caelo	Cinnamon, cut	13304401	2
Caelo	Cinnamon, cut	13304402	2
Caelo	Cinnamon, cut	25111307	1
Caelo	Cinnamon, cut	12309902	3
Caelo	Cinnamon, cut	12309908	1
Caelo	Cinnamon, cut	11357912	2
Caelo	Cinnamon, cut	13304407	1
Caelo	Clove	13371309	1
Caelo	Clove	14057602	1
Caelo	Clove	12266505	1
Caelo	Clove	12095806	2
Caelo	Clove	5398872	1
Caelo	Clove	12095807	5
Caelo	Clove	11233305	1
Caelo	Clove	12095802	1
Caelo	Clove, powdered (spice)	14180001	1
Caelo	Clove, powdered (spice)	12355303	1
Caelo	Cocaine hydrochloride	13259306	1
Caelo	Cocaine hydrochloride	13112102	1
Caelo	Cocaine hydrochloride	12329103	1
Caelo	Cocaine hydrochloride	17003902	2
Caelo	Cocaine hydrochloride	16051402	1
Caelo	Cocaine hydrochloride	14069209	1
Caelo	Cocoa bark, cut	19011303	1
Caelo	Cocoa bark, cut	12126907	1
Caelo	Cocoa bark, cut	1216907	1
Caelo	Cocoa bark, cut	12126905	2
Caelo	Cocoa bark, cut	12126910	1
Caelo	Cocoa bark, cut	12126901	1
Caelo	Codeine phosphate hem...	16349706	2
Caelo	Codeine phosphate hem...	14275910	1
Caelo	Codeine phosphate hem...	18187903	1
Caelo	Codeine phosphate hem...	13I27-N06	1
Caelo	Codeine phosphate hem...	15219805	2
Caelo	Codeine phosphate hem...	1427910	1
Caelo	Codeine phosphate hem...	15350703	2
Caelo	Coltsfoot leaf, cut	Int.Ch:Now16081	1
Caelo	Coltsfoot leaf, cut	2021B130319	3

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Supplier	Substance	Batch	Spectra
Caelo	Coltsfoot leaf, cut	23041302	1
Caelo	Comfrey root	2711Q-02135	1
Caelo	Comfrey root	116053	1
Caelo	Common broom herb, cut	12358804	3
Caelo	Common broom herb, cut	12358802	1
Caelo	Common broom herb, cut	13241601	1
Caelo	Common broom herb, cut	11132209	1
Caelo	Common broom herb, cut	4412Q-01680	1
Caelo	Common broom herb, cut	12358805	1
Caelo	Common wormwood herb,...	12016708	5
Caelo	Common wormwood herb,...	12382701	6
Caelo	Common wormwood herb,...	12016711	3
Caelo	Common wormwood herb,...	12016705	5
Caelo	Common wormwood herb,...	3591A110119	4
Caelo	Common wormwood herb,...	1081301	1
Caelo	Common wormwood herb,...	18031302	1
Caelo	Common wormwood herb,...	1238701	1
Caelo	Common wormwood herb,...	10355329	1
Caelo	Common wormwood herb,...	9355403	1
Caelo	Common wormwood herb,...	12382706	1
Caelo	Common wormwood herb,...	12382705	2
Caelo	Common wormwood herb,...	12016707	3
Caelo	Common wormwood herb,...	14360605	1
Caelo	Common wormwood herb,...	12016702	1
Caelo	Common wormwood herb,...	12382702	10
Caelo	Common wormwood herb,...	12016709	2
Caelo	Copper (II) sulfate p...	3211M-01317	1
Caelo	Copper (II) sulfate p...	12157107	1
Caelo	Copper (II) sulfate p...	10L15-N06	1
Caelo	Copper (II) sulfate p...	3411M-01317	1
Caelo	Copper (II) sulfate p...	2913U-01317	1
Caelo	Coriander	12080905	1
Caelo	Coriander	16010201	1
Caelo	Coriander	9285707	1
Caelo	Coriander	4091305	1
Caelo	Coriander	27061305	1
Caelo	Coriander	13010304	1
Caelo	Coriander	13010302	2
Caelo	Coriander	12080906	1
Caelo	Coriander	14031316	1
Caelo	Coriander	12080901	2
Caelo	Coriander	13010306	2
Caelo	Coriander	16010209	1
Caelo	Cottonwood bud	12027506	1
Caelo	Cottonwood bud	12027504	1
Caelo	Cottonwood bud	70864257	1
Caelo	Couch grass rhizome, ...	10049618	2
Caelo	Couch grass rhizome, ...	10349705	1
Caelo	Couch grass rhizome, ...	10349704	1
Caelo	Couch grass rhizome, ...	3712I-02180	1
Caelo	Couch grass rhizome, ...	12186817	3
Caelo	Couch grass rhizome, ...	12186705	1
Caelo	Couch grass rhizome, ...	10049614	1
Caelo	Cowberry leaf, cut	12105201	1
Caelo	Cowberry leaf, cut	11334302	1
Caelo	Cowberry leaf, cut	12105203	1
Caelo	Cowberry leaf, cut	12150205	1
Caelo	Daisy flower	12133705	1
Caelo	Daisy flower	1210a120215	2
Caelo	Daisy flower	11103203	2

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Supplier	Substance	Batch	Spectra
Caelo	Daisy flower	11068308	1
Caelo	Daisy flower	11103201	2
Caelo	Daisy flower	12133703	1
Caelo	Damiana leaf, cut	12064103	3
Caelo	Damiana leaf, cut	12330401	4
Caelo	Damiana leaf, cut	12330403	2
Caelo	Damiana leaf, cut	11026607	2
Caelo	Damiana leaf, cut	12330407	2
Caelo	Damiana leaf, cut	12330402	7
Caelo	Dandelion herb with r...	11030313	2
Caelo	Dandelion herb with r...	11030311	2
Caelo	Dandelion herb with r...	806212165	1
Caelo	Dandelion herb with r...	10121602	1
Caelo	Dandelion herb with r...	11030309	2
Caelo	Dandelion herb with r...	Ch.-B.:13019802	1
Caelo	Dandelion herb with r...	11371903	1
Caelo	Dandelion herb with r...	13019805	1
Caelo	Dandelion herb with r...	6611B100902	1
Caelo	Dandelion herb with r...	13018902	1
Caelo	Dandelion herb with r...	13019801	5
Caelo	Dandelion herb with r...	11030314	4
Caelo	Dandelion herb with r...	13019802	19
Caelo	Dandelion herb with r...	8111205	1
Caelo	Dandelion herb with r...	12236003	3
Caelo	Dandelion herb with r...	1103011	1
Caelo	Dandelion herb with r...	20111202	1
Caelo	Dandelion herb with r...	12236002	8
Caelo	Dandelion herb with r...	2112122165	1
Caelo	Dandelion herb with r...	12236005	5
Caelo	Dandelion herb with r...	11030305	1
Caelo	Dandelion herb with r...	Int.Ch:318090	1
Caelo	Dandelion herb with r...	7341703	1
Caelo	Dandelion herb with r...	13108801	4
Caelo	Dandelion herb with r...	12236001	3
Caelo	Dandelion herb with r...	13317903	1
Caelo	Dandelion herb with r...	17121305	1
Caelo	Dandelion herb with r...	13199202	2
Caelo	Dandelion herb with r...	13019802-3395310101	1
Caelo	Dandelion herb with r...	13108802	11
Caelo	Dandelion herb withou...	13091305	1
Caelo	Dandelion herb withou...	11217107	1
Caelo	Dandelion herb withou...	11030311	1
Caelo	Dandelion herb withou...	1127102	1
Caelo	Dandelion herb withou...	7031305	1
Caelo	Dandelion herb withou...	9011403	1
Caelo	Dandelion herb withou...	11371904	2
Caelo	Dandelion herb withou...	11217109	1
Caelo	Dandelion herb withou...	107063	1
Caelo	Dandelion herb withou...	1137907	1
Caelo	Dandelion herb withou...	11371907	1
Caelo	Dandelion herb withou...	11371902	1
Caelo	Dandelion root, cut	12367916	1
Caelo	Dandelion root, cut	12363109	2
Caelo	Dandelion root, cut	12363108	2
Caelo	Dandelion root, cut	16161303	1
Caelo	Dandelion root, cut	12363107	1
Caelo	Dandelion root, cut	16161308	1
Caelo	Dandelion root, cut	13329702	8
Caelo	Dandelion root, cut	12363110	1
Caelo	Dandelion root, cut	13329705	1

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Supplier	Substance	Batch	Spectra
Caelo	Dandelion root, cut	11003313	1
Caelo	Dandelion root, cut	12363106	1
Caelo	Dandelion root, cut	12363102	2
Caelo	Dandelion root, cut	12363104	3
Caelo	Dandelion root, cut	10024710	1
Caelo	Dandelion root, cut	1140317	1
Caelo	Dandelion root, cut	15407703	1
Caelo	Dandelion root, cut	14166501	1
Caelo	Dandelion root, cut	15407703	1
Caelo	Dandelion root, cut	11003307	1
Caelo	Dandelion root, cut	11003311	2
Caelo	Dandelion root, cut	14166504	1
Caelo	Dandelion root, cut	14376602	1
Caelo	Dandelion root, cut	14376603	1
Caelo	Dandelion root, cut	12363103	1
Caelo	Dandelion root, cut	14166502	1
Caelo	Devil's claw root	6331B110426	2
Caelo	Devil's claw root	12031811	1
Caelo	Devil's claw root	12031810	1
Caelo	Devil's claw root	12031803	1
Caelo	Devil's claw root	12031806	1
Caelo	Dexamphetamine sulfate	C9H13N14	1
Caelo	Dihydrocodeine hydrog...	12142503	2
Caelo	Dihydrocodeine hydrog...	12142508	2
Caelo	Dihydrocodeine hydrog...	13267603	1
Caelo	Dihydrocodeine hydrog...	13267604	2
Caelo	Dihydrocodeine hydrog...	13267608	1
Caelo	Dihydrocodeine hydrog...	15295903	2
Caelo	Dihydrocodeine hydrog...	15295905	2
Caelo	Dihydrocodeine hydrog...	15F18-B07-322054	1
Caelo	Dihydrocodeine hydrog...	15295907	1
Caelo	Dill fruit	12342901	2
Caelo	Dill fruit	12038304	4
Caelo	Dill fruit	12289901	1
Caelo	Dill fruit	12342904	6
Caelo	Dill fruit	9189003	1
Caelo	Dill fruit	12342906	2
Caelo	Dill fruit	16040406	1
Caelo	Dill fruit	12342903	1
Caelo	Dill fruit	12038302	2
Caelo	Dill fruit	12342909	5
Caelo	Dill fruit	12342908	2
Caelo	Dill herb, cut	13007601	1
Caelo	Dill herb, cut	13007602	1
Caelo	Dill herb, cut	13007605	1
Caelo	Dill herb, cut	13007608	1
Caelo	Dill herb, cut	11295109	1
Caelo	Dill herb, cut	15178603	1
Caelo	Dry beads Caelo ora...	11005811	1
Caelo	Echinacea pallida roo...	12244504	1
Caelo	Echinacea pallida roo...	11115206	1
Caelo	Econazole nitrate	ECN140301	1
Caelo	Elder berries	12267801	1
Caelo	Elder flower, rubbed	13244601	4
Caelo	Elder flower, rubbed	5122013d	1
Caelo	Elder flower, rubbed	12221910	2
Caelo	Elder flower, rubbed	14111317	1
Caelo	Elder flower, rubbed	13244602	2
Caelo	Elder flower, rubbed	10291310	5
Caelo	Elder flower, rubbed	12221907	4

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Supplier	Substance	Batch	Spectra
Caelo	Elder flower, rubbed	12221906	1
Caelo	Elder flower, rubbed	1571A121022	14
Caelo	Elder flower, rubbed	1571a121022	1
Caelo	Elder flower, rubbed	10291309	3
Caelo	Elder flower, rubbed	12221902	10
Caelo	Elder flower, rubbed	1029310	1
Caelo	Elder flower, rubbed	12221905	7
Caelo	Elder flower, rubbed	10291312	2
Caelo	Elder flower, rubbed	12221904	10
Caelo	Elder flower, rubbed	12221904-3360319071	1
Caelo	Elder flower, rubbed	10291308	2
Caelo	Elder flower, rubbed	31051301	1
Caelo	Elecampane rhizome, cut	12113304	3
Caelo	Elecampane rhizome, cut	1211334	1
Caelo	Elecampane rhizome, cut	12113303	1
Caelo	Elecampane rhizome, cut	11374703	1
Caelo	Elecampane rhizome, cut	11374702	1
Caelo	Elecampane rhizome, cut	13152403	2
Caelo	Elecampane rhizome, cut	13152402	1
Caelo	Elecampane rhizome, cut	13152401	1
Caelo	Eleutherococcus, cut	10381817	1
Caelo	Eleutherococcus, cut	12326707	1
Caelo	Eleutherococcus, cut	10381818	2
Caelo	Eleutherococcus, cut	12326703	1
Caelo	Eleutherococcus, cut	12326701	1
Caelo	Elm bark, cut	10347203	1
Caelo	Elm bark, cut	12287902	2
Caelo	Elm bark, cut	10347204	1
Caelo	Equisetum stem, cut	10328915	1
Caelo	Equisetum stem, cut	6081304	1
Caelo	Equisetum stem, cut	10375507	2
Caelo	Equisetum stem, cut	11021901	1
Caelo	Equisetum stem, cut	11076302	2
Caelo	Equisetum stem, cut	13344305	1
Caelo	Equisetum stem, cut	13159702-3464312101	1
Caelo	Equisetum stem, cut	8041301	1
Caelo	Equisetum stem, cut	13200201	1
Caelo	Equisetum stem, cut	8051302	1
Caelo	Equisetum stem, cut	30101305	1
Caelo	Equisetum stem, cut	13159705-3387310190	1
Caelo	Equisetum stem, cut		2
Caelo	Equisetum stem, cut	9101313	1
Caelo	Equisetum stem, cut	13159704	6
Caelo	Equisetum stem, cut	13091301	1
Caelo	Equisetum stem, cut	13159706	5
Caelo	Equisetum stem, cut	13153702	1
Caelo	Equisetum stem, cut	1359702	1
Caelo	Equisetum stem, cut	13159705	6
Caelo	Equisetum stem, cut	12288808	8
Caelo	Equisetum stem, cut	12288809	3
Caelo	Equisetum stem, cut	13159702	8
Caelo	Equisetum stem, cut	12288802	2
Caelo	Equisetum stem, cut	282573	1
Caelo	Equisetum stem, cut	2011408	1
Caelo	Equisetum stem, cut	311042	1
Caelo	Equisetum stem, cut	13344303	6
Caelo	Equisetum stem, cut	3091201	1
Caelo	Equisetum stem, cut	11076306	6
Caelo	Equisetum stem, cut	8101201	1
Caelo	Equisetum stem, cut	17101203	1

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Supplier	Substance	Batch	Spectra
Caelo	Equisetum stem, cut	11021904	1
Caelo	Equisetum stem, cut	13344306	1
Caelo	Equisetum stem, cut	11076303	12
Caelo	Equisetum stem, cut	11076307	1
Caelo	Equisetum stem, cut	12288804	11
Caelo	Equisetum stem, cut	10375520	1
Caelo	Equisetum stem, cut	2658181	1
Caelo	Equisetum stem, cut	20111212	1
Caelo	Equisetum stem, cut	1288804	1
Caelo	Equisetum stem, cut	10328901	1
Caelo	Equisetum stem, cut	13344309	3
Caelo	Equisetum stem, cut	13344302	3
Caelo	Equisetum stem, cut	15015404	1
Caelo	Equisetum stem, cut	13350309	1
Caelo	Equisetum stem, cut	13344304	5
Caelo	Equisetum stem, cut	13350301	1
Caelo	Equisetum stem, cut	13344311	1
Caelo	Eucalyptus leaf, cut	122250204	1
Caelo	Eucalyptus leaf, cut	12225202	1
Caelo	Eucalyptus leaf, cut	12225203	3
Caelo	Eucalyptus leaf, cut	12225206	1
Caelo	Eucalyptus leaf, cut	11307708	2
Caelo	Eucalyptus leaf, cut	9346811	1
Caelo	Euphrasy herb, cut	8011419	1
Caelo	Euphrasy herb, cut	112211643	1
Caelo	Euphrasy herb, cut	11030810	1
Caelo	Euphrasy herb, cut	29011302	1
Caelo	Euphrasy herb, cut	12103202	9
Caelo	Euphrasy herb, cut	11030812	4
Caelo	Euphrasy herb, cut	13180008	1
Caelo	Euphrasy herb, cut	12103203	9
Caelo	Euphrasy herb, cut	1213202	1
Caelo	Euphrasy herb, cut	312052	1
Caelo	Euphrasy herb, cut	13180001	5
Caelo	Euphrasy herb, cut	13180002	4
Caelo	Euphrasy herb, cut	14019102	2
Caelo	Euphrasy herb, cut	13180004	5
Caelo	Euphrasy herb, cut	12103201	1
Caelo	Euphrasy herb, cut	13180005	2
Caelo	Euphrasy herb, cut	14019107	1
Caelo	Euphrasy herb, cut	30101307	1
Caelo	Euphrasy herb, cut	7051302	1
Caelo	Euphrasy herb, cut	11030811	3
Caelo	European golden rod, ...	12343102	1
Caelo	European golden rod, ...	12343103-3466312121	1
Caelo	European golden rod, ...	13386908	1
Caelo	Fenugreek	12252601	2
Caelo	Fenugreek	12252602	2
Caelo	Fenugreek	11313203	1
Caelo	Fenugreek	12252603	2
Caelo	Fenugreek	13013801	1
Caelo	Fenugreek	13013803	6
Caelo	Fenugreek	1131206	1
Caelo	Fenugreek	13013805	3
Caelo	Fenugreek, powdered	15308703	2
Caelo	Fenugreek, powdered	14057807	1
Caelo	Fenugreek, powdered	14057801	1
Caelo	Fenugreek, powdered	14377201	2
Caelo	Fenugreek, powdered	13398302	1
Caelo	Fenugreek, powdered	12149607	1

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Supplier	Substance	Batch	Spectra
Caelo	Fenugreek, powdered	12149605	1
Caelo	Fenugreek, powdered	7264a110201	2
Caelo	Feverfew herb, cut	12380203	5
Caelo	Feverfew herb, cut	12380204	1
Caelo	Flax weed herb, cut	16292801	1
Caelo	Flax weed herb, cut	14005305	3
Caelo	Flax weed herb, cut	14005303	1
Caelo	Flax weed herb, cut	13007507	7
Caelo	Flax weed herb, cut	13007505	1
Caelo	Flax weed herb, cut	11104505	1
Caelo	Flax weed herb, cut	13007502	2
Caelo	Flax weed herb, cut	11104507	8
Caelo	Flax weed herb, cut	14197204	1
Caelo	Frangula bark, cut	6011402	1
Caelo	Frangula bark, cut	12186002	15
Caelo	Frangula bark, cut	12186003	1
Caelo	Frangula bark, cut	10061301	1
Caelo	Frangula bark, cut	eztetdt	1
Caelo	Frangula bark, cut	12186004	11
Caelo	Frangula bark, cut	1286003	1
Caelo	Frangula bark, cut	12185901	9
Caelo	Frangula bark, cut	13203008	1
Caelo	Frangula bark, cut	12186006	6
Caelo	Frangula bark, cut	11340801	1
Caelo	Frangula bark, cut	121860006	1
Caelo	Frangula bark, cut	11254001	2
Caelo	Frangula bark, cut	12186005	1
Caelo	Frangula bark, cut	12186001	1
Caelo	Frangula bark, cut	14163102	1
Caelo	Frankincense	15140804	1
Caelo	Frankincense	14107803	2
Caelo	Frankincense	4614M-02030	1
Caelo	Frankincense	15140809	1
Caelo	Frankincense	12120012-3421310191	1
Caelo	Frankincense	15140810	1
Caelo	Frankincense	15140805	2
Caelo	Frankincense	13112809	2
Caelo	Frankincense	13112803	1
Caelo	Frankincense	13112807	1
Caelo	Frankincense	12120008	2
Caelo	Frankincense	13112803-3494411030	1
Caelo	Frankincense	12120006	3
Caelo	Frankincense	12120005	5
Caelo	Frankincense	10349213	1
Caelo	Frankincense	10349210	1
Caelo	Frankincense	13112801	5
Caelo	Fumitory, cut	11101411	3
Caelo	Fumitory, cut	11101410	1
Caelo	Fumitory, cut	11101406	1
Caelo	Fumitory, cut	13202905	2
Caelo	Fumitory, cut	1320902	1
Caelo	Fumitory, cut	12103407	6
Caelo	Fumitory, cut	12103408	5
Caelo	Fumitory, cut	13202902	11
Caelo	Fumitory, cut	8312901	1
Caelo	Fumitory, cut	72878477	1
Caelo	Fumitory, cut	7111201	1
Caelo	Fumitory, cut	11101413	3
Caelo	Fumitory, cut	12103405	7
Caelo	Fumitory, cut	12103404	2

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Supplier	Substance	Batch	Spectra
Caelo	Fumitory, cut	11101408	1
Caelo	Galangal root	12125004	2
Caelo	Galangal root	1215004	1
Caelo	Galangal root	11375904	1
Caelo	Galangal root	12330303	1
Caelo	Galangal root	12330305	1
Caelo	Galangal root	12330306	2
Caelo	Galangal root	15128008	1
Caelo	Garden violet, cut	10011403	1
Caelo	Garden violet, cut	11124008	1
Caelo	Garden violet, cut	11124007-3284310662	1
Caelo	Garden violet, cut	13038701	4
Caelo	Garden violet, cut	13232107	1
Caelo	Garden violet, cut	11124007	1
Caelo	Garden violet, cut	1303872	1
Caelo	Garden violet, cut	13038703	2
Caelo	Gentian root, cut	10263404	1
Caelo	Gentian root, cut	6311B130305	2
Caelo	Gentian root, cut	30011301	1
Caelo	Gentian root, cut	19071304	1
Caelo	Gentian root, cut	Int.Ch:313091	1
Caelo	Gentian root, cut	12244608	1
Caelo	Gentian root, cut	12244607	1
Caelo	Gentian root, cut	10263411	1
Caelo	Gentian root, cut	13156102	1
Caelo	Gentian root, powdered	12007106	1
Caelo	Gentian root, powdered	15011403	1
Caelo	Gentian root, powdered	14215601	1
Caelo	Ginger, peeled	11325712	1
Caelo	Ginger, peeled	19121201	1
Caelo	Ginger, peeled	11325715	2
Caelo	Ginger, peeled	11325719	3
Caelo	Ginger, peeled	11325716	1
Caelo	Ginger, peeled	13100602	2
Caelo	Ginger, peeled	11325703	2
Caelo	Ginger, peeled	12164911-3368319002	1
Caelo	Ginger, peeled	13100604	1
Caelo	Ginger, peeled	13310602	2
Caelo	Ginger, peeled	13310604	3
Caelo	Ginger, peeled	12180604	1
Caelo	Ginger, peeled	13100605	3
Caelo	Ginger, peeled, powde...	12164911	1
Caelo	Ginger, peeled, powde...	13092013B	1
Caelo	Ginger, peeled, powde...	12164901	1
Caelo	Ginkgo leaf, cut	12373604	1
Caelo	Ginkgo leaf, cut	13340906	1
Caelo	Ginkgo leaf, cut	12151709	2
Caelo	Ginkgo leaf, cut	13340904	1
Caelo	Ginkgo leaf, cut	15077407	1
Caelo	Ginkgo leaf, cut	13340907	1
Caelo	Ginseng root	13341001	1
Caelo	Ginseng root	12080218	1
Caelo	Goat's rue, cut	12343305	3
Caelo	Goat's rue, cut	12343302	4
Caelo	Goat's rue, cut	11175104	1
Caelo	Goat's rue, cut	5122013e	1
Caelo	Goat's rue, cut	12343308	1
Caelo	Goat's rue, cut	12343303	6
Caelo	Goat's rue, cut	12017914	1
Caelo	Goat's rue, cut	12017912	1

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Supplier	Substance	Batch	Spectra
Caelo	Goat's rue, cut	12017907	3
Caelo	Goat's rue, cut	11307901	1
Caelo	Goat's rue, cut	12017913	1
Caelo	Goat's rue, cut	11307903	1
Caelo	Ground ivy herb, cut	11374615	1
Caelo	Ground ivy herb, cut	11374611	1
Caelo	Ground ivy herb, cut	11052315	1
Caelo	Ground ivy herb, cut	11374602	1
Caelo	Ground ivy herb, cut	11052318	2
Caelo	Ground ivy herb, cut	11374606	1
Caelo	Ground ivy herb, cut	11052314	1
Caelo	Ground ivy herb, cut	11374609	1
Caelo	Guaiacum wood, cut	11352001	1
Caelo	Guaiacum wood, cut	11352008	1
Caelo	Guaiacum wood, cut	11352012	1
Caelo	Guaiacum wood, cut	8041401	1
Caelo	Guaiacum wood, cut	14008203	1
Caelo	Guaiacum wood, cut	16136706	1
Caelo	Guaiacum wood, cut	16136710	1
Caelo	Guaiacum wood, cut	4011M-01778	1
Caelo	Guaiacum wood, cut	11352010	1
Caelo	Hamamelis bark, cut	13123701	1
Caelo	Hamamelis bark, cut	13123703	1
Caelo	Hamamelis bark, cut	12361301	1
Caelo	Hamamelis leaf, cut	10102915	1
Caelo	Hamamelis leaf, cut	12164804	1
Caelo	Hamamelis leaf, cut	12165805	1
Caelo	Hamamelis leaf, cut	14356103	1
Caelo	Hamamelis leaf, cut	13269902	2
Caelo	Hamamelis leaf, cut	12164802	1
Caelo	Hamamelis leaf, cut	13269904	1
Caelo	Hamamelis leaf, cut	13269905	1
Caelo	Hawthorn flower	11068206	1
Caelo	Hawthorn flower	13010402	3
Caelo	Hawthorn flower	11068209	1
Caelo	Hawthorn flower	13010402	2
Caelo	Hawthorn flower	13010403	4
Caelo	Hawthorn flower	25101301	1
Caelo	Hawthorn flower	11068208	1
Caelo	Hawthorn flower	1351B130819	3
Caelo	Hawthorn flower	13253303	1
Caelo	Hawthorn flower	13253304	1
Caelo	Hawthorn flower	7121201	1
Caelo	Hawthorn flower	11068202	1
Caelo	Hawthorn flower	21051301	1
Caelo	Hawthorn fruit	13367203	1
Caelo	Hawthorn fruit	13101402	1
Caelo	Hawthorn fruit	12326306	1
Caelo	Hawthorn fruit	12326307	2
Caelo	Hawthorn fruit	12326308	1
Caelo	Hawthorn fruit	12326304	1
Caelo	Hawthorn fruit	11278202	1
Caelo	Hawthorn leaf with fl...	12225107	5
Caelo	Hawthorn leaf with fl...	16025802	1
Caelo	Hawthorn leaf with fl...	2225104	1
Caelo	Hawthorn leaf with fl...	12225108	7
Caelo	Hawthorn leaf with fl...	12225104	12
Caelo	Hawthorn leaf with fl...	11068206	1
Caelo	Hawthorn leaf with fl...	IntCh: 313082	1
Caelo	Hawthorn leaf with fl...	1221707	1

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Supplier	Substance	Batch	Spectra
Caelo	Hawthorn leaf with fl...	52467476	1
Caelo	Hawthorn leaf with fl...	15188802	1
Caelo	Hawthorn leaf with fl...	13276703	3
Caelo	Hawthorn leaf with fl...	12225207	1
Caelo	Hawthorn leaf with fl...	11366001	1
Caelo	Hawthorn leaf with fl...	10273515	6
Caelo	Hawthorn leaf with fl...	1225107	1
Caelo	Hawthorn leaf with fl...	1518802	1
Caelo	Hawthorn leaf with fl...	10273512	2
Caelo	Hawthorn leaf with fl...	109076	1
Caelo	Hawthorn leaf with fl...	1222514	1
Caelo	Hay flower	13097301	1
Caelo	Hay flower	11099902	1
Caelo	Hay flower	11099912	1
Caelo	Hay flower	25101202	1
Caelo	Hay flower	11099914	1
Caelo	Hay flower	11099916	1
Caelo	Hay flower	11099915	1
Caelo	Hay flower	11099909	1
Caelo	Hay flower	12317101	7
Caelo	Hay flower	12317104	10
Caelo	Hay flower	12317102	2
Caelo	Hay flower	3713F-01459	1
Caelo	Hay flower	14121301	1
Caelo	Hay flower	13099205	1
Caelo	Hay flower	13097302	7
Caelo	Hay flower	12317110	2
Caelo	Hay flower	12371707	1
Caelo	Hay flower	12317107	11
Caelo	Hay flower	3713E-01459	1
Caelo	Hay flower	12317108	3
Caelo	Heather flower, rubbed	10270516	1
Caelo	Heather flower, rubbed	13014204	4
Caelo	Heather flower, rubbed	13014206	1
Caelo	Heather, cut	9291512	1
Caelo	Heather, cut	11011209	2
Caelo	Heather, cut	19111203	1
Caelo	Heather, cut	28061201	1
Caelo	Heather, cut	11102901	1
Caelo	Heather, cut	13367502	1
Caelo	Heavy alkaline bismut...	12146911	3
Caelo	Heavy alkaline bismut...	12146913	2
Caelo	Heavy alkaline bismut...	12146902	1
Caelo	Heavy alkaline bismut...	4513M-01186	1
Caelo	Heavy alkaline bismut...	12146903	4
Caelo	Heavy alkaline bismut...	10F09-N13	1
Caelo	Heavy alkaline bismut...	10013208	1
Caelo	Heavy alkaline bismut...	11052805	1
Caelo	Heavy alkaline bismut...	10013213	1
Caelo	Heavy alkaline bismut...	11052809	1
Caelo	Heavy alkaline bismut...	M468105	1
Caelo	Henna powder	12122310	3
Caelo	Henna powder	13262803	2
Caelo	Henna powder	12267311	1
Caelo	Hop strobile	12008313	2
Caelo	Hop strobile	1451b120817	1
Caelo	Hop strobile	12221802	2
Caelo	Hop strobile	12008309	2
Caelo	Hop strobile	12092001	2
Caelo	Hop strobile	12008310	3

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Supplier	Substance	Batch	Spectra
Caelo	Hop strobile	12008310	3
Caelo	Hop strobile	12008307	1
Caelo	Hop strobile	12006305	1
Caelo	Hop strobile	15061211	1
Caelo	Hop strobile	12008305	1
Caelo	Hop strobile	12008302	1
Caelo	Hop strobile	120008312	1
Caelo	Hop strobile	12008317	6
Caelo	Hop strobile	13123804	3
Caelo	Hop strobile	12380101	6
Caelo	Hop strobile	13123803	1
Caelo	Hop strobile	30121301	1
Caelo	Hop strobile	13123807	1
Caelo	Hop strobile	13123803-3505411011	1
Caelo	Hop strobile	4111304	1
Caelo	Hop strobile	4756769	1
Caelo	Hop strobile	13187602	1
Caelo	Hop strobile	12221807	1
Caelo	Hop strobile	13123804-3563412081	1
Caelo	Hop strobile	13123803	7
Caelo	Hop strobile	12008315	1
Caelo	Hop strobile	6091303	1
Caelo	Hop strobile	10240308	1
Caelo	Hop strobile	13123806	1
Caelo	Hop strobile	13123802	8
Caelo	Hop strobile	14068007	1
Caelo	Hop strobile	13123802	3
Caelo	Hop strobile	12221805	3
Caelo	Hop strobile	1451B130107	6
Caelo	Hop strobile	12380103	1
Caelo	Hop strobile	12008317	1
Caelo	Hop strobile	131223805	1
Caelo	Hop strobile	12221804	1
Caelo	Hop strobile	5021306	1
Caelo	Horse chestnut leaf, ...	11063503	2
Caelo	Hydromorphone hydroch...	16273604	1
Caelo	Hydromorphone hydroch...	16123805	2
Caelo	Hydromorphone hydroch...	15393605	1
Caelo	Hydromorphone hydroch...	14210405	1
Caelo	Hyssop herb, cut	11374304	1
Caelo	Hyssop herb, cut	13143902	1
Caelo	Iceland moss, cut	12187002	1
Caelo	Iceland moss, cut	13350803	4
Caelo	Iceland moss, cut	12382806	1
Caelo	Iceland moss, cut	15297601	1
Caelo	Iceland moss, cut	13350805	4
Caelo	Iceland moss, cut	11101601	1
Caelo	Iceland moss, cut	11101607	8
Caelo	Iceland moss, cut	12187102	18
Caelo	Iceland moss, cut	12197002	1
Caelo	Iceland moss, cut	4912E-01774	1
Caelo	Iceland moss, cut	11053911	1
Caelo	Iceland moss, cut	15297603	1
Caelo	Iceland moss, cut	12187107	1
Caelo	Iceland moss, cut	11053916	1
Caelo	Iceland moss, cut	13350807	4
Caelo	Iceland moss, cut	9052804	2
Caelo	Iceland moss, cut	14304402	1
Caelo	Iceland moss, cut	14304401	1
Caelo	Iceland moss, cut	14304403	2

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Supplier	Substance	Batch	Spectra
Caelo	Iceland moss, cut	12187106	2
Caelo	Iceland moss, cut	15297605	1
Caelo	Iceland moss, cut	1287102	1
Caelo	Iceland moss, cut	12187108	4
Caelo	Iceland moss, cut	14304407	2
Caelo	Iceland moss, cut	12187109	4
Caelo	Iceland moss, cut	12187103	1
Caelo	Iceland moss, cut	14304409	5
Caelo	Iron (III) sulfate hy...	10354404	1
Caelo	Iron (III) sulfate hy...	10354412	1
Caelo	Iron (III) sulfate hy...	12175906	1
Caelo	Iron (III) sulfate hy...	1512210007	1
Caelo	Iron (III) sulfate hy...	10354415	1
Caelo	Iron (III) sulfate hy...	12175908	1
Caelo	Ispaghula seed	12276501	2
Caelo	Ispaghula seed	16121302	1
Caelo	Ispaghula seed	26011401	1
Caelo	Ispaghula seed	14031408	1
Caelo	Ispaghula seed	11061405	1
Caelo	Ispaghula seed	4114001	1
Caelo	Ispaghula seed	12276527	1
Caelo	Ispaghula seed	23011505	1
Caelo	Ispaghula seed	14246602	3
Caelo	Ispaghula seed	142660	1
Caelo	Ispaghula seed	15081503	1
Caelo	Ispaghula seed	29061510	1
Caelo	Ispaghula seed	4121201	1
Caelo	Ispaghula seed	11185811	2
Caelo	Ispaghula seed	18061804	1
Caelo	Ispaghula seed	28111703	1
Caelo	Ispaghula seed	8041702	1
Caelo	Ispaghula seed	15249315	1
Caelo	Ispaghula seed	15121901	1
Caelo	Ispaghula seed	15249319	2
Caelo	Ispaghula seed	30101302	1
Caelo	Ispaghula seed	4121202	1
Caelo	Ispaghula seed	5091319	1
Caelo	Ispaghula seed	10011303	1
Caelo	Ispaghula seed	413E-03369	1
Caelo	Ispaghula seed	12276511	1
Caelo	Ispaghula seed	3051302	1
Caelo	Ispaghula seed	12252709	1
Caelo	Ispaghula seed	1227506	1
Caelo	Ispaghula seed	18071301	1
Caelo	Ispaghula seed	19061308	1
Caelo	Ispaghula seed	9011302	1
Caelo	Ivy leaf, cut	4011301	1
Caelo	Ivy leaf, cut	11229505	5
Caelo	Ivy leaf, cut	2031301	1
Caelo	Ivy leaf, cut	8061205	1
Caelo	Ivy leaf, cut	11101205	1
Caelo	Ivy leaf, cut	12225603	2
Caelo	Ivy leaf, cut	11041303	1
Caelo	Ivy leaf, cut	12225602	1
Caelo	Ivy leaf, cut	27111301	1
Caelo	Ivy leaf, cut	23121305	1
Caelo	Ivy leaf, cut	10011401	1
Caelo	Ivy leaf, cut	12225605	5
Caelo	Ivy leaf, cut	23121303	1
Caelo	Ivy leaf, cut	20111211	1

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Supplier	Substance	Batch	Spectra
Caelo	Ivy leaf, cut	15101203	1
Caelo	Jasmine flower	12143203	3
Caelo	Java tea, cut	2221A110825	2
Caelo	Java tea, cut	20111207	1
Caelo	Java tea, cut	31121203	1
Caelo	Java tea, cut	2221B121112	14
Caelo	Java tea, cut	12225702	1
Caelo	Java tea, cut	12225704	2
Caelo	Java tea, cut	21061304	1
Caelo	Java tea, cut	13258802	2
Caelo	Java tea, cut	28101305	1
Caelo	Java tea, cut	13258804	3
Caelo	Java tea, cut	11212901	1
Caelo	Juniper	2890a101201	2
Caelo	Juniper	12330505	1
Caelo	Juniper, pounded	14149502	1
Caelo	Juniper, pounded	13031302	1
Caelo	Juniper, pounded	13367302	1
Caelo	Kaolin, heavy	10176518	1
Caelo	Kaolin, heavy	11350125	4
Caelo	Kaolin, heavy	11350124	2
Caelo	Kaolin, heavy	11350107	1
Caelo	Kaolin, heavy	82043269	1
Caelo	Kaolin, heavy	13041803	1
Caelo	Kaolin, heavy	13041803	1
Caelo	Kaolin, heavy	13041835	1
Caelo	Kaolin, heavy	13041835	1
Caelo	Kaolin, heavy	11041610	1
Caelo	Kaolin, heavy	63033516	1
Caelo	Kelp, cut	11352209	1
Caelo	Kelp, cut	280172	4
Caelo	Kelp, cut	11351109	1
Caelo	Kelp, cut	14071502	1
Caelo	Kidney vetch, coarsel...	13104301	2
Caelo	Knotgrass, cut	12368903	1
Caelo	Knotgrass, cut	12295702	3
Caelo	Knotgrass, cut	12295704	4
Caelo	Knotgrass, cut	12368902	5
Caelo	Knotgrass, cut	4312M-01674	1
Caelo	Knotgrass, cut	7102427	1
Caelo	Knotgrass, cut	12368904	1
Caelo	Knotgrass, cut	12368906	3
Caelo	Knotgrass, cut	14079304	1
Caelo	Knotgrass, cut	8111202	1
Caelo	Knotgrass, cut	4301A100126	2
Caelo	Ladys bedstraw herb,...	10375707	2
Caelo	Ladys bedstraw herb,...	15029906	1
Caelo	Ladys bedstraw herb,...	10375702	1
Caelo	Ladys bedstraw herb,...	24101201	1
Caelo	Ladys bedstraw herb,...	11265103	5
Caelo	Ladys bedstraw herb,...	11265102	8
Caelo	Ladys bedstraw herb,...	7011301	1
Caelo	Ladys bedstraw herb,...	2401311647	1
Caelo	Ladys bedstraw herb,...	14019202	1
Caelo	Ladys bedstraw herb,...	11265104	1
Caelo	Ladys bedstraw herb,...	11265106	1
Caelo	Ladys bedstraw herb,...	12369001	3
Caelo	Ladys bedstraw herb,...	12369002	3
Caelo	Ladys bedstraw herb,...	12369007	3
Caelo	Ladys bedstraw herb,...	12369006	5

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Supplier	Substance	Batch	Spectra
Caelo	Ladys bedstraw herb,...	22041303	1
Caelo	Lapacho wood, cut	2x11154506	1
Caelo	Lapacho wood, cut	12239303	2
Caelo	Lapacho wood, cut	11154506	1
Caelo	Lapacho wood, cut	13298305	1
Caelo	Lapacho wood, cut	13298308	1
Caelo	Lapacho wood, cut	12239305	8
Caelo	Lapacho wood, cut	19061301	1
Caelo	Large waybread herb, ...	12374104	7
Caelo	Large waybread herb, ...	13232401	1
Caelo	Large waybread herb, ...	123741004	1
Caelo	Large waybread herb, ...	10349614	1
Caelo	Large waybread herb, ...	12374101	4
Caelo	Large waybread herb, ...	12374106	1
Caelo	Large waybread herb, ...	9311208	1
Caelo	Large waybread herb, ...	10349610	1
Caelo	Large waybread herb, ...	14125907	1
Caelo	Large waybread herb, ...	10349603	2
Caelo	Large waybread herb, ...	13232404	1
Caelo	Laurel leaf	12299106	3
Caelo	Laurel leaf	12299101	1
Caelo	Lavender flower	1318501	1
Caelo	Lavender flower	13185006	1
Caelo	Lavender flower	13185001-3415310152	1
Caelo	Lavender flower	13159601	1
Caelo	Lavender flower	13185001-3389311070	1
Caelo	Lavender flower	13336008	1
Caelo	Lavender flower	13387204	1
Caelo	Lavender flower	13185002	1
Caelo	Lavender flower	12088005	3
Caelo	Lavender flower	13185001	27
Caelo	Lavender flower	11054104	2
Caelo	Lavender flower	11054106	2
Caelo	Lavender flower	11054107	1
Caelo	Lavender flower	15061201	1
Caelo	Lavender flower	15061209	1
Caelo	Lavender flower	11327903	5
Caelo	Lavender flower	6091304	1
Caelo	Lavender flower	11327905	2
Caelo	Lavender flower	12088002	4
Caelo	Lavender flower	12031302	1
Caelo	Lavender flower	12088006	3
Caelo	Lavender flower	13185003	10
Caelo	Lavender flower	19071303	1
Caelo	Lavender flower	27091202	1
Caelo	Lavender flower	12088003	8
Caelo	Lemon grass, cut	11301501	1
Caelo	Lemon grass, cut	11301503	1
Caelo	Lemon grass, cut	11301509	2
Caelo	Lemon grass, cut	13341301	1
Caelo	Lemon grass, cut	13149703	1
Caelo	Lemon grass, cut	13149701	4
Caelo	Lemon peel, cut	12217401	1
Caelo	Lemon peel, cut	12217402	1
Caelo	Lemon peel, cut	12217404	1
Caelo	Lemon verbena leaf, cut	12137505	1
Caelo	Lemon verbena leaf, cut	12137507	3
Caelo	Lemon verbena leaf, cut	13037702	1
Caelo	Lemon verbena leaf, cut	10018208	1
Caelo	Lime flower, cut	10273606	1

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Supplier	Substance	Batch	Spectra
Caelo	Lime flower, cut	12170702	2
Caelo	Lime flower, cut	28031302	1
Caelo	Lime flower, cut	Int.Ch:210140	1
Caelo	Lime flower, cut	12170701	1
Caelo	Lime flower, cut	13337403-348012102	1
Caelo	Lime flower, cut	11086305	7
Caelo	Lime flower, cut	15111301	1
Caelo	Lime flower, cut	13337403	5
Caelo	Lime flower, cut	15068302	1
Caelo	Lime flower, cut	13101702	7
Caelo	Lime flower, cut	13101708	1
Caelo	Lime flower, cut	12170702-3355319071	1
Caelo	Lime flower, cut	13101701	7
Caelo	Lime flower, cut	1210702	1
Caelo	Lime flower, cut	9206604	1
Caelo	Lime flower, cut	268709	2
Caelo	Lime flower, cut	12170703	1
Caelo	Lime flower, cut	272958	7
Caelo	Lime flower, cut	10273608	2
Caelo	Lime flower, cut	11086307	3
Caelo	Lime leaf, cut	1611A121120	1
Caelo	Linseed	11199006	1
Caelo	Linseed	13262702	1
Caelo	Linseed	15061201	1
Caelo	Linseed	12092102	4
Caelo	Linseed	12186901	2
Caelo	Linseed	11199003	1
Caelo	Linseed	11365508	1
Caelo	Linseed	12092103	3
Caelo	Linseed	12321604	2
Caelo	Linseed	12321601	1
Caelo	Linseed	12092104	2
Caelo	Linseed	12382002	2
Caelo	Linseed	28051303	1
Caelo	Linseed	12321606	2
Caelo	Linseed	18111302	1
Caelo	Linseed	12321607	1
Caelo	Linseed	12382006	3
Caelo	Linseed	12321602	4
Caelo	Linseed	1232006	1
Caelo	Linseed	11365507	1
Caelo	Linseed	12382004	1
Caelo	Linseed	4713U02240	1
Caelo	Linseed	13296702	3
Caelo	Linseed	1326703	2
Caelo	Linseed	7370A131104	1
Caelo	Linseed	13140305	1
Caelo	Linseed	13412804	1
Caelo	Linseed	13296705	5
Caelo	Linseed	13262704	2
Caelo	Linseed	7307A141201	2
Caelo	Linseed	15006601	2
Caelo	Linseed	15053702	1
Caelo	Linseed	15006602	1
Caelo	Linseed	15006005	1
Caelo	Linseed	15006605	1
Caelo	Linseed	15006607	1
Caelo	Linseed	15321902	1
Caelo	Linseed	3615A-02240	1
Caelo	Linseed	16040001	1

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Supplier	Substance	Batch	Spectra
Caelo	Linseed	16011403	2
Caelo	Linseed	16040002	1
Caelo	Linseed	16011405	1
Caelo	Linseed	16040005	1
Caelo	Linseed	21081703	1
Caelo	Linseed	7307A170619	2
Caelo	Linseed	17067204	1
Caelo	Linseed	28051403	1
Caelo	Linseed	13262703	3
Caelo	Linseed	13296707	1
Caelo	Liquorice root, peeled	1135904	1
Caelo	Liquorice root, peeled	13194101	5
Caelo	Liquorice root, peeled	10011301	1
Caelo	Liquorice root, peeled	1351911	1
Caelo	Liquorice root, peeled	11351911	4
Caelo	Liquorice root, peeled	11351913	1
Caelo	Liquorice root, peeled	11351910	2
Caelo	Liquorice root, peeled	638a120806	1
Caelo	Liquorice root, peeled	11351905	3
Caelo	Liquorice root, peeled	12227112	1
Caelo	Liquorice root, peeled	6381A111004	14
Caelo	Liquorice root, peeled	277004	1
Caelo	Liquorice root, peeled	13104503	3
Caelo	Liquorice root, peeled	18121302	1
Caelo	Liquorice root, peeled	13104504	4
Caelo	Liquorice root, natur...	13037902	1
Caelo	Liquorice root, natur...		1
Caelo	Liquorice root, natur...	12267103	1
Caelo	Liquorice root, natur...	12267104	2
Caelo	Liquorice root, natur...	13037904	1
Caelo	Liquorice root, natur...	10110912	1
Caelo	Lovage root, cut	12189001	1
Caelo	Lovage root, cut	11181611	3
Caelo	Lovage root, cut	12169008	4
Caelo	Lovage root, cut	13385005	1
Caelo	Lovage root, cut	12169012	1
Caelo	Lovage root, cut	12169010	2
Caelo	Lovage root, cut	107063	1
Caelo	Lovage root, cut	12169009	1
Caelo	Lovage root, cut	12169006	3
Caelo	Lovage root, cut	11181609	3
Caelo	Lovage root, cut	4312M-02150	1
Caelo	Lovage root, cut	12169002	2
Caelo	Lovage root, cut	12189002	1
Caelo	Lungwort herb, cut	11134203	12
Caelo	Lungwort herb, cut	11021707	1
Caelo	Lungwort herb, cut	11134202	3
Caelo	Lungwort herb, cut	13029302	23
Caelo	Lungwort herb, cut	11134205	3
Caelo	Lungwort herb, cut	11134201	1
Caelo	Lungwort herb, cut	13029306	2
Caelo	Lungwort herb, cut	13355801	2
Caelo	Lungwort herb, cut	4331b111205	1
Caelo	Lungwort herb, cut	11021709	2
Caelo	Lycopodium herb, cut	11255016	1
Caelo	Lycopodium herb, cut	11255018	1
Caelo	Lycopodium herb, cut	13101501	1
Caelo	Lycopodium herb, cut	11255017	6
Caelo	Lycopodium herb, cut	11255010	1
Caelo	Lycopodium herb, cut	11255012	2

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Supplier	Substance	Batch	Spectra
Caelo	Lycopodium herb, cut	11255014	7
Caelo	Lycopodium herb, cut	9378812	1
Caelo	Lycopodium herb, cut	11255003	1
Caelo	Lycopodium herb, cut	11255005	3
Caelo	Lycopodium herb, cut	11255008	12
Caelo	Lycopodium herb, cut	11255011	5
Caelo	Lycopodium herb, cut	1310502	1
Caelo	Lycopodium herb, cut	11255009	2
Caelo	Magnesium carbonate, ...	7011404	1
Caelo	Magnesium carbonate, ...	2091303	1
Caelo	Magnesium carbonate, ...	12135404	1
Caelo	Magnesium carbonate, ...	13123502	1
Caelo	Magnesium carbonate, ...	13123504	2
Caelo	Magnesium carbonate, ...	13123505	1
Caelo	Magnesium chloride he...	12354615	8
Caelo	Magnesium chloride he...	12354612	6
Caelo	Magnesium chloride he...	12141808	1
Caelo	Magnesium chloride he...	11345624	1
Caelo	Magnesium chloride he...	12354618	2
Caelo	Magnesium chloride he...	12354608	1
Caelo	Magnesium chloride he...	5210I-01828	1
Caelo	Magnesium chloride he...	12141803	1
Caelo	Magnesium chloride he...	16094004	1
Caelo	Magnesium chloride he...	12141807	3
Caelo	Magnesium chloride he...	12354613	4
Caelo	Magnesium chloride he...	12354610	2
Caelo	Magnesium chloride he...	1108024-01	1
Caelo	Magnesium chloride he...	11345623	1
Caelo	Magnesium chloride he...	13194702	3
Caelo	Magnesium chloride he...	13194706	3
Caelo	Magnesium chloride he...	13194721	2
Caelo	Magnesium chloride he...	1304C004	2
Caelo	Magnesium chloride he...	1021401	1
Caelo	Magnesium chloride he...	13194707	4
Caelo	Magnesium chloride he...	13194713	1
Caelo	Magnesium chloride he...	13194701	1
Caelo	Magnesium chloride he...	13194713-3490312103	1
Caelo	Magnesium chloride he...	12141811	2
Caelo	Magnesium chloride he...	12141817	2
Caelo	Magnesium chloride he...	12354605	4
Caelo	Magnesium chloride he...	11345609	1
Caelo	Magnesium chloride he...	12141814	1
Caelo	Magnesium chloride he...	12354604	4
Caelo	Magnesium chloride he...	1512I-01828	1
Caelo	Magnesium chloride he...	12354606	4
Caelo	Magnesium chloride he...	12354609	6
Caelo	Magnesium chloride he...	12141806	2
Caelo	Magnesium chloride he...	11345606	1
Caelo	Magnesium sulfate hep...	13030107	1
Caelo	Magnesium sulfate hep...	90744129	1
Caelo	Magnesium sulfate hep...	11369509	1
Caelo	Magnesium sulfate hep...	12119901/2	1
Caelo	Magnesium sulfate hep...	11369525	6
Caelo	Magnesium sulfate hep...	11194001	1
Caelo	Magnesium sulfate hep...	12336915	3
Caelo	Magnesium sulfate hep...	11369529	1
Caelo	Magnesium sulfate hep...	11369526	13
Caelo	Magnesium sulfate hep...	10371111	1
Caelo	Magnesium sulfate hep...	12336914	5
Caelo	Magnesium sulfate hep...	10104201	1

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Supplier	Substance	Batch	Spectra
Caelo	Magnesium sulfate hep...	13183702	2
Caelo	Magnesium sulfate hep...	1213E-01835	1
Caelo	Magnesium sulfate hep...	6012014B	1
Caelo	Magnesium sulfate hep...	113695625	1
Caelo	Magnesium sulfate hep...	12336926	1
Caelo	Magnesium sulfate hep...	12138521	4
Caelo	Magnesium sulfate hep...	11369252	1
Caelo	Magnesium sulfate hep...	13030104	1
Caelo	Magnesium sulfate hep...	1206019-01	5
Caelo	Magnesium sulfate hep...	12c27-n06	1
Caelo	Magnesium sulfate, dr...	11265902	1
Caelo	Magnesium sulfate, dr...	12157202	1
Caelo	Magnesium sulfate, dr...	10213213	2
Caelo	Magnesium sulfate, dr...	M-220413-2	1
Caelo	Magnesium sulfate, dr...	12157208	1
Caelo	Magnesium sulfate, dr...	11265903	1
Caelo	Magnesium sulfate, dr...	11265908	2
Caelo	Magnesium sulfate, dr...	12157207	1
Caelo	Maize style, cut	10325905	1
Caelo	Maize style, cut	280363	1
Caelo	Maize style, cut	10325904	1
Caelo	Maize style, cut	10325907	2
Caelo	Maize style, cut	13277205	1
Caelo	Maize style, cut	13277202	1
Caelo	Maize style, cut	13277201	1
Caelo	Maize style, cut	10325906	7
Caelo	Maize style, cut	13277207	1
Caelo	Maize style, cut	11280404	2
Caelo	Maize style, cut	10325902	2
Caelo	Maize style, cut	11280405	9
Caelo	Male speedwell wort, ...	4661c111011	1
Caelo	Male speedwell wort, ...	3051306	1
Caelo	Male speedwell wort, ...	12162504	12
Caelo	Male speedwell wort, ...	11061305	1
Caelo	Male speedwell wort, ...	28061303	1
Caelo	Male speedwell wort, ...	12162505	2
Caelo	Male speedwell wort, ...	3091305	1
Caelo	Male speedwell wort, ...	13166701	3
Caelo	Male speedwell wort, ...	14111303	1
Caelo	Male speedwell wort, ...	12162503	1
Caelo	Male speedwell wort, ...	20111303	1
Caelo	Male speedwell wort, ...	1216504	1
Caelo	Male speedwell wort, ...	11265502	1
Caelo	Male speedwell wort, ...	11265503	5
Caelo	Mallow flower, cut	12187501	6
Caelo	Mallow flower, cut	12187502	1
Caelo	Mallow flower, cut	12187505	3
Caelo	Mallow flower, cut	10357904	1
Caelo	Mallow flower, cut	12187404	4
Caelo	Mallow flower, cut	10357902	1
Caelo	Mallow flower, cut	20061201	1
Caelo	Mallow flower, cut	11040106	4
Caelo	Mallow flower, cut	9311104	1
Caelo	Mallow flower, cut	27021301	1
Caelo	Mallow flower, cut	13040402	1
Caelo	Mallow flower, cut	12187405	4
Caelo	Mallow flower, cut	13267301-3409310112	1
Caelo	Mallow flower, cut	12187501-3414310132	1
Caelo	Mallow flower, cut	18111303	1
Caelo	Mallow flower, cut	13267303	2

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Supplier	Substance	Batch	Spectra
Caelo	Mallow flower, cut	13267302	1
Caelo	Mallow flower, cut	13351301	2
Caelo	Mallow flower, cut	13351303	2
Caelo	Mallow flower, cut	13351309	1
Caelo	Mallow flower, cut	13351307	1
Caelo	Mallow flower, cut	8121202	1
Caelo	Mallow leaf, cut	20111302	1
Caelo	Mallow leaf, cut	13174213	1
Caelo	Mallow leaf, cut	12310008	1
Caelo	Mallow leaf, cut	14073902	1
Caelo	Mallow leaf, cut	13174207	1
Caelo	Mallow leaf, cut	13174217	1
Caelo	Mallow leaf, cut	2131B120529	3
Caelo	Mallow leaf, cut	10290515	1
Caelo	Mallow leaf, cut	12310001	2
Caelo	Mallow leaf, cut	12310004	4
Caelo	Mallow leaf, cut	28061203	1
Caelo	Mallow leaf, cut	12153403	1
Caelo	Mallow leaf, cut	10290502	1
Caelo	Mallow leaf, cut	12310006	1
Caelo	Mallow leaf, cut	12310009	2
Caelo	Manna, cut	11308911	2
Caelo	Manna, cut	14001303	3
Caelo	Manna, cut	28101404	1
Caelo	Manna, cut	11308907	2
Caelo	Manna, cut	25071403	1
Caelo	Manna, cut	14001310	3
Caelo	Manna, cut	11308901	2
Caelo	Manna, cut	15219003	2
Caelo	Manna, cut	13127003	5
Caelo	Manna, cut	25111301	1
Caelo	Manna, cut	11041401	1
Caelo	Manna, cut	11308909	2
Caelo	Manna, cut	11061404	1
Caelo	Manna, cut	13041712	1
Caelo	Manna, cut	15219008	2
Caelo	Manna, cut	15111738	1
Caelo	Manna, cut	15219010	2
Caelo	Manna, cut	15219005	1
Caelo	Manna, powdered	15101306	1
Caelo	Manna, powdered	11071311	1
Caelo	Manna, powdered	11003611	1
Caelo	Manna, powdered	15101312	1
Caelo	Manna, powdered	11308807	1
Caelo	Manna, powdered	14001402	1
Caelo	Manna, powdered	14001408	1
Caelo	Manna, powdered	11308802	2
Caelo	Marian thistle fruit	12189107	2
Caelo	Marian thistle fruit	11126705	1
Caelo	Marian thistle fruit	11126702	9
Caelo	Marian thistle fruit	10270613	1
Caelo	Marian thistle fruit	12189104	2
Caelo	Marian thistle fruit	12189106	4
Caelo	Marian thistle fruit	27111203	1
Caelo	Marian thistle fruit	12189108	4
Caelo	Marian thistle fruit	1126703	1
Caelo	Marian thistle fruit	15409204	2
Caelo	Marian thistle fruit	11126703	1
Caelo	Marian thistle fruit	13326202	3
Caelo	Marian thistle fruit	10270614	2

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Supplier	Substance	Batch	Spectra
Caelo	Marian thistle fruit	12189116	2
Caelo	Marian thistle fruit	18111301	1
Caelo	Marian thistle fruit	12189115	2
Caelo	Marian thistle fruit	12189111	3
Caelo	Marian thistle fruit	12189112	5
Caelo	Marian thistle fruit	12198107	1
Caelo	Marian thistle fruit	11126701	1
Caelo	Marian thistle fruit	1289112	1
Caelo	Marian thistle fruit	12189113	6
Caelo	Marian thistle fruit	12189109	2
Caelo	Marian thistle fruit	12189105	1
Caelo	Marian thistle fruit	1126705	1
Caelo	Marian thistle herb, ...	18041303	1
Caelo	Marian thistle herb, ...	10365605	1
Caelo	Marian thistle herb, ...	10315907	1
Caelo	Marian thistle herb, ...	17121204	1
Caelo	Marian thistle herb, ...	62607127	1
Caelo	Marian thistle herb, ...	1313702	1
Caelo	Marian thistle herb, ...	13130702	3
Caelo	Marian thistle herb, ...	10365601	4
Caelo	Marian thistle herb, ...	10365604	3
Caelo	Marian thistle herb, ...	1035911	1
Caelo	Marian thistle herb, ...	30101306	1
Caelo	Marian thistle herb, ...	10315911	3
Caelo	Marian thistle herb, ...	13130704	5
Caelo	Marian thistle herb, ...	13130701	2
Caelo	Marian thistle herb, ...	13386703-3543411013	1
Caelo	Marian thistle herb, ...	intch:318080	1
Caelo	Marian thistle herb, ...	13130703	2
Caelo	Marian thistle herb, ...	13130701-3492411030	1
Caelo	Marian thistle herb, ...	10315909	1
Caelo	Marjoram herb, rubbed	12168906	1
Caelo	Marjoram herb, rubbed	12168905	2
Caelo	Marjoram herb, rubbed	9292602	1
Caelo	Marjoram herb, rubbed	12168904	1
Caelo	Marjoram herb, rubbed	12168902	1
Caelo	Marjoram herb, rubbed	11212711	3
Caelo	Marjoram herb, rubbed	12168908	6
Caelo	Marjoram herb, rubbed	12168910	8
Caelo	Marjoram herb, rubbed	12168903	9
Caelo	Marjoram herb, rubbed	12168909	5
Caelo	Marjoram herb, rubbed	27011402	1
Caelo	Marjoram herb, rubbed	13113304	3
Caelo	Marjoram herb, rubbed	13113303	3
Caelo	Marjoram herb, rubbed	12168912	1
Caelo	Marjoram herb, rubbed	12168901	3
Caelo	Marjoram herb, rubbed	12168907	3
Caelo	Marjoram herb, rubbed	6051302	1
Caelo	Marrubium vulgare her...	12231604	4
Caelo	Marrubium vulgare her...	12231601	3
Caelo	Marrubium vulgare her...	12231603	1
Caelo	Marrubium vulgare her...	313091	1
Caelo	Marrubium vulgare her...	1153803	1
Caelo	Marrubium vulgare her...	11253802	1
Caelo	Marrubium vulgare her...	13289109	1
Caelo	Marrubium vulgare her...	11253803	1
Caelo	Marrubium vulgare her...	12231605	4
Caelo	Marshmallow leaf, cut	12328207	2
Caelo	Marshmallow leaf, cut	13199604	4
Caelo	Marshmallow leaf, cut	12328206	3

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Supplier	Substance	Batch	Spectra
Caelo	Marshmallow leaf, cut	12328202	3
Caelo	Marshmallow root, nat...	270114	1
Caelo	Marshmallow root, pee...	11101907	7
Caelo	Marshmallow root, pee...	12147311	1
Caelo	Marshmallow root, pee...	12147311	6
Caelo	Marshmallow root, pee...	11101804	1
Caelo	Marshmallow root, pee...	6071A130116	10
Caelo	Marshmallow root, pee...	11101804	1
Caelo	Marshmallow root, pee...	26091201	1
Caelo	Marshmallow root, pee...	11101905	1
Caelo	Marshmallow root, pee...	13057103	1
Caelo	Marshmallow root, pee...	12368906	1
Caelo	Marshmallow root, pee...	15104503	1
Caelo	Masterwort root, cut	13341201	1
Caelo	Masterwort root, cut	12101808	1
Caelo	Masterwort root, cut	12101806	2
Caelo	Masterwort root, cut	1210801	1
Caelo	Masterwort root, cut	13132002	1
Caelo	Masterwort root, cut	12101807	2
Caelo	Maté leaf, cut	13061202	1
Caelo	Maté leaf, cut	12133804	7
Caelo	Maté leaf, cut	11091710	1
Caelo	Maté leaf, cut	12133803	3
Caelo	Maté leaf, cut	12133807	7
Caelo	Maté leaf, cut	2141A120821	2
Caelo	Maté leaf, cut	13118001	1
Caelo	Maté leaf, cut	12133806	1
Caelo	Maté leaf, cut	13118003	4
Caelo	Maté leaf, cut	12133801	3
Caelo	Matricaria flower	13210906	1
Caelo	Matricaria flower	12361707	2
Caelo	Matricaria flower	12337608	1
Caelo	Matricaria flower	11101203	1
Caelo	Matricaria flower	13210905	3
Caelo	Matricaria flower	13210901-3478312171	1
Caelo	Matricaria flower	12294804	1
Caelo	Matricaria flower	13210903	1
Caelo	Matricaria flower	12361706	1
Caelo	Matricaria flower	13011406	1
Caelo	Matricaria flower	13210905	1
Caelo	Matricaria flower	13288405	3
Caelo	Matricaria flower	13210901	3
Caelo	Matricaria flower	12361706	3
Caelo	Matricaria flower	12361702	6
Caelo	Matricaria flower	12361707	4
Caelo	Matricaria flower	22011303	1
Caelo	Matricaria flower	12244805	4
Caelo	Matricaria flower	12244803	1
Caelo	Matricaria flower	12244804	2
Caelo	Matricaria flower	12299701	1
Caelo	Matricaria flower	22111202	1
Caelo	Matricaria flower	22111201	1
Caelo	Matricaria flower	12244802	4
Caelo	Matricaria flower	19111207	1
Caelo	Matricaria flower	16111202	1
Caelo	Matricaria flower	13111201	1
Caelo	Matricaria flower	12111903	2
Caelo	Matricaria flower	27091203	1
Caelo	Matricaria flower	12244803	3
Caelo	Matricaria flower	17101204	1

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Supplier	Substance	Batch	Spectra
Caelo	Matricaria flower	12059606	2
Caelo	Matricaria flower	12361704	1
Caelo	Matricaria flower	12294802	15
Caelo	Matricaria flower	20021313	1
Caelo	Matricaria flower	AKD5	1
Caelo	Matricaria flower	12337610	1
Caelo	Matricaria flower	26081303	1
Caelo	Matricaria flower	11214810	1
Caelo	Matricaria flower	IntCh:313011	1
Caelo	Matricaria flower	12337607	2
Caelo	Matricaria flower	12337601	1
Caelo	Matricaria flower	13210901-3546411013	1
Caelo	Matricaria flower	11218501	1
Caelo	Matricaria flower	11169607	1
Caelo	Matricaria flower	13061201	1
Caelo	Matricaria flower	12361701	3
Caelo	Matricaria flower	19041306	1
Caelo	Matricaria flower	10081201	1
Caelo	Matricaria flower	22081202	1
Caelo	Matricaria flower	12299703	2
Caelo	Matricaria flower	13031306	1
Caelo	Matricaria flower	5081201	1
Caelo	Matricaria flower	15090003	2
Caelo	Matricaria flower	14276804	3
Caelo	Matricaria flower	15258504	1
Caelo	Matricaria flower	15258505	1
Caelo	Meadowsweet flower, r...	12275704-3372319032	1
Caelo	Meadowsweet flower, r...	12275703	3
Caelo	Meadowsweet flower, r...	9326211	2
Caelo	Meadowsweet flower, r...	12275704	4
Caelo	Meadowsweet flower, r...	10349302	2
Caelo	Meadowsweet flower, r...	10349307	2
Caelo	Meadowsweet flower, r...	10051301	1
Caelo	Meadowsweet flower, r...	12275701	2
Caelo	Meadowsweet flower, r...	1227501	1
Caelo	Meadowsweet flower, r...	10349305	1
Caelo	Meadowsweet flower, r...	1225702	1
Caelo	Meadowsweet flower, r...	9326213	2
Caelo	Meadowsweet herb, cut	62487517	1
Caelo	Meadowsweet herb, cut	12188801	1
Caelo	Meadowsweet herb, cut	12188807	1
Caelo	Meadowsweet herb, cut	12188806	3
Caelo	Meadowsweet herb, cut	10381602	3
Caelo	Meadowsweet herb, cut	12188703	1
Caelo	Meadowsweet herb, cut	12188805	12
Caelo	Meadowsweet herb, cut	12188704	2
Caelo	Meadowsweet herb, cut	12188702	1
Caelo	Meadowsweet herb, cut	10381601	1
Caelo	Meadowsweet herb, cut	12188803	9
Caelo	Meadowsweet herb, cut	4912E-01685	1
Caelo	Melilot herb, cut	107063	1
Caelo	Melilot herb, cut	8061204	1
Caelo	Melilot herb, cut	11307601	1
Caelo	Melilot herb, cut	11307607	1
Caelo	Melilot herb, cut	12289203	5
Caelo	Melilot herb, cut	25091301	1
Caelo	Melilot herb, cut	12289205	3
Caelo	Melilot herb, cut	22111303	1
Caelo	Melilot herb, cut	12289201	1
Caelo	Melilot herb, cut	12289206	1

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Supplier	Substance	Batch	Spectra
Caelo	Melilot herb, cut	12289207	1
Caelo	Melilot herb, cut	12231703	3
Caelo	Melilot herb, cut	19071201	1
Caelo	Melilot herb, cut	11307606	6
Caelo	Melilot herb, cut	12231701	3
Caelo	Melilot herb, cut	12289202	8
Caelo	Melilot herb, cut	24081202	1
Caelo	Melissa leaf, cut	12032318	1
Caelo	Melissa leaf, cut	14111319	1
Caelo	Melissa leaf, cut	12032309	1
Caelo	Melissa leaf, cut	13030805	1
Caelo	Melissa leaf, cut	25061303	1
Caelo	Melissa leaf, cut	13030803	2
Caelo	Melissa leaf, cut	2161a121009	1
Caelo	Melissa leaf, cut		1
Caelo	Melissa leaf, cut	19041303	1
Caelo	Melissa leaf, cut	12032319	5
Caelo	Melissa leaf, cut	25021301	1
Caelo	Melissa leaf, cut	1009	1
Caelo	Melissa leaf, cut	24011407	1
Caelo	Melissa leaf, cut	12032316	3
Caelo	Melissa leaf, cut	CH. 111111	1
Caelo	Melissa leaf, cut	13214707	1
Caelo	Melissa leaf, cut	13214720	1
Caelo	Melissa leaf, cut	12032307	2
Caelo	Melissa leaf, cut	10310919	1
Caelo	Melissa leaf, cut	12032310	1
Caelo	Melissa leaf, cut	12032303	1
Caelo	Melissa leaf, cut	13214705	1
Caelo	Methadone hydrochloride	16135318	3
Caelo	Methadone hydrochloride	1723509	1
Caelo	Methadone hydrochloride	13266514	1
Caelo	Methadone hydrochloride	1613529	1
Caelo	Methadone hydrochloride	16135315	1
Caelo	Methadone hydrochloride	13266501	1
Caelo	Methadone hydrochloride	171920-0004	1
Caelo	Methadone hydrochloride	17239514	1
Caelo	Methadone hydrochloride	15244704	4
Caelo	Methadone hydrochloride	13266515	1
Caelo	Methadone hydrochloride	13266518	3
Caelo	Methadone hydrochloride	13266505	4
Caelo	Methadone hydrochloride	1081801	1
Caelo	Methadone hydrochloride	20170728/Ma2	1
Caelo	Methadone hydrochloride	13266511	2
Caelo	Methadone hydrochloride	16135325	1
Caelo	Methadone hydrochloride	15244702	1
Caelo	Methadone hydrochloride	16135329	4
Caelo	Methadone hydrochloride	16135326	4
Caelo	Methadone hydrochloride	16135327	5
Caelo	Methadone hydrochloride	16135325,170814MHC	1
Caelo	Methadone hydrochloride	16135317	1
Caelo	Methadone hydrochloride	15244715	2
Caelo	Methadone hydrochloride	16135310	4
Caelo	Methadone hydrochloride	13266521	1
Caelo	Methadone hydrochloride	15244713	4
Caelo	Methadone hydrochloride	15244717	6
Caelo	Methadone hydrochloride	1723	1
Caelo	Methadone hydrochloride	15215501	1
Caelo	Methadone hydrochloride	17239518	1
Caelo	Methadone hydrochloride	23021802	1

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Supplier	Substance	Batch	Spectra
Caelo	Methadone hydrochloride	15244701	1
Caelo	Methadone hydrochloride	15244709	2
Caelo	Methadone hydrochloride	16135302	1
Caelo	Methadone hydrochloride	15244710	4
Caelo	Methadone hydrochloride	15244718	1
Caelo	Methadone hydrochloride	15I24-B07-317266	1
Caelo	Methadone hydrochloride	1327H051	1
Caelo	Methadone hydrochloride	14C24-B01-292860	1
Caelo	Methadone hydrochloride	16135307	2
Caelo	Methadone hydrochloride	16135303	1
Caelo	Methadone hydrochloride	16135305	6
Caelo	Methadone hydrochloride	16135301	1
Caelo	Methadone hydrochloride	28041725	1
Caelo	Methadone hydrochloride	10076407	1
Caelo	Methadone hydrochloride	16135308	2
Caelo	Methadone hydrochloride	15244705	1
Caelo	Methadone hydrochloride	17239503	2
Caelo	Methadone hydrochloride	16F24-B02-323184	1
Caelo	Methadone hydrochloride	16135312	3
Caelo	Methadone hydrochloride	15244706	3
Caelo	Methadone hydrochloride	16135311	4
Caelo	Methadone hydrochloride	28061702	1
Caelo	Methadone hydrochloride	15244720	1
Caelo	Methadone hydrochloride	12344802	1
Caelo	Methadone hydrochloride	13266502	2
Caelo	Methadone hydrochloride	17239504	3
Caelo	Methadone hydrochloride	12171902	1
Caelo	Methadone hydrochloride	25111701	1
Caelo	Methadone hydrochloride	13266504	2
Caelo	Methadone hydrochloride	17239506	2
Caelo	Methadone hydrochloride	17239502	3
Caelo	Methadone hydrochloride	17239507	3
Caelo	Methadone hydrochloride	3111806	1
Caelo	Methadone hydrochloride	1729504	1
Caelo	Methadone hydrochloride	180219MC/17239506	1
Caelo	Methadone hydrochloride	17C24-B05	2
Caelo	Methadone hydrochloride	12171914	1
Caelo	Methadone hydrochloride	16135330	2
Caelo	Methadone hydrochloride	16135323	1
Caelo	Methadone hydrochloride	18132403	1
Caelo	Methadone hydrochloride	17239501	1
Caelo	Methadone hydrochloride	19011913	1
Caelo	Methadone hydrochloride	31011901	1
Caelo	Methadone hydrochloride	18132408	1
Caelo	Methadone hydrochloride	17239510	1
Caelo	Methadone hydrochloride	16135324	1
Caelo	Methadone hydrochloride	17I15-B02-339523	2
Caelo	Methadone hydrochloride	2912161	1
Caelo	Methadone hydrochloride	12171907	1
Caelo	Methadone hydrochloride	172329504	1
Caelo	Methadone hydrochloride	16135328	1
Caelo	Methadone hydrochloride	12344814	2
Caelo	Methadone hydrochloride	17011406	1
Caelo	Methadone hydrochloride	18186604	1
Caelo	Methadone hydrochloride	12344818	1
Caelo	Methadone hydrochloride	12344816	3
Caelo	Methadone hydrochloride	12171918	1
Caelo	Methadone hydrochloride	12344812	2
Caelo	Methadone hydrochloride	12344819	1
Caelo	Methadone hydrochloride	12344807	1

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Supplier	Substance	Batch	Spectra
Caelo	Methadone hydrochloride	17051801	1
Caelo	Methadone hydrochloride	12171906	2
Caelo	Methadone hydrochloride	7091708	1
Caelo	Methadone hydrochloride	17239512	3
Caelo	Methadone hydrochloride	16135332	5
Caelo	Methadone hydrochloride	18186601	1
Caelo	Methadone hydrochloride	11227507	1
Caelo	Methylrosanilinium ch...	9238106	1
Caelo	Methylrosanilinium ch...	12H28-N06	1
Caelo	Methylrosanilinium ch...	9238107	1
Caelo	Methylrosanilinium ch...	12/17-N05	1
Caelo	Methylrosanilinium ch...	12H28-No6	1
Caelo	Methylrosanilinium ch...	13184801	1
Caelo	Midazolam hydrochloride	14339009	1
Caelo	Midazolam hydrochloride	11184705	1
Caelo	Midazolam hydrochloride	15224603	1
Caelo	Midazolam hydrochloride	14339015	1
Caelo	Midazolam hydrochloride	15224605	1
Caelo	Midazolam hydrochloride	16290605	2
Caelo	Midazolam hydrochloride	15224607	2
Caelo	Midazolam hydrochloride	83600116001	1
Caelo	Midazolam hydrochloride	15224614	1
Caelo	Midazolam hydrochloride	14339002	1
Caelo	Midazolam hydrochloride	17168003	2
Caelo	Midazolam hydrochloride	15224616	2
Caelo	Mistletoe, cut	10273412	1
Caelo	Mistletoe, cut	29061201	1
Caelo	Mistletoe, cut	10081205	1
Caelo	Mistletoe, cut	10091201	1
Caelo	Mistletoe, cut	10273407	1
Caelo	Mistletoe, cut	23111204	1
Caelo	Mistletoe, cut	11294003	2
Caelo	Mistletoe, cut	11266702	4
Caelo	Mistletoe, cut	10273418	1
Caelo	Mistletoe, cut	11266703	3
Caelo	Mistletoe, cut	6061306	1
Caelo	Mistletoe, cut	17061304	1
Caelo	Mistletoe, cut	26071302	1
Caelo	Mistletoe, cut	29071302	1
Caelo	Mistletoe, cut	11294004	5
Caelo	Mistletoe, cut	29081302	1
Caelo	Mistletoe, cut	11294005	15
Caelo	Mistletoe, cut	3813E-01695	1
Caelo	Mistletoe, cut	4313E-01695	1
Caelo	Mistletoe, cut	28101304	1
Caelo	Mistletoe, cut	29101302	1
Caelo	Mistletoe, cut	11266712-3450311162	1
Caelo	Mistletoe, cut	11266713	2
Caelo	Mistletoe, cut	20121303	1
Caelo	Mistletoe, cut	27121305	1
Caelo	Mistletoe, cut	24011401	1
Caelo	Mistletoe, cut	14292506	2
Caelo	Mistletoe, cut	14292514	1
Caelo	Mistletoe, cut	11266712	8
Caelo	Mistletoe, cut	11266709	9
Caelo	Mistletoe, cut	11266714	4
Caelo	Mistletoe, cut	10273420	5
Caelo	Mistletoe, cut	18031303	1
Caelo	Mistletoe, cut	11266704	14
Caelo	Mistletoe, cut	11266705	3

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Supplier	Substance	Batch	Spectra
Caelo	Mistletoe, cut	12011301	1
Caelo	Mistletoe, cut	11266710	7
Caelo	Mistletoe, cut	11266708	8
Caelo	Mistletoe, cut	11021303	1
Caelo	Molecular distilled g...	11160012	1
Caelo	Morphine hydrochloride	15199705	1
Caelo	Morphine hydrochloride	15199705Nr. 2	1
Caelo	Morphine hydrochloride	14081701	1
Caelo	Morphine hydrochloride	16184607	1
Caelo	Morphine hydrochloride	14055084	1
Caelo	Morphine hydrochloride	12104409	1
Caelo	Morphine hydrochloride	15199711	4
Caelo	Morphine hydrochloride	15439405	2
Caelo	Morphine hydrochloride	1543904	1
Caelo	Morphine hydrochloride	14238619	1
Caelo	Morphine hydrochloride	15439409	1
Caelo	Morphine hydrochloride	13125208	1
Caelo	Morphine hydrochloride	15199705Nr. 3	1
Caelo	Morphine hydrochloride	12318101	1
Caelo	Morphine hydrochloride	15439402	1
Caelo	Morphine hydrochloride	16184614	1
Caelo	Morphine hydrochloride	13125206	1
Caelo	Morphine hydrochloride	12104403	1
Caelo	Morphine hydrochloride	15199713	1
Caelo	Morphine hydrochloride	14238604	1
Caelo	Morphine hydrochloride	16184613	6
Caelo	Morphine hydrochloride	15199707	1
Caelo	Morphine hydrochloride	13081310	1
Caelo	Morphine hydrochloride	16184610	1
Caelo	Morphine hydrochloride	14238617	1
Caelo	Motherwort herb, cut	5061203	1
Caelo	Motherwort herb, cut	12376403	1
Caelo	Motherwort herb, cut	11293004	1
Caelo	Motherwort herb, cut	12376407	1
Caelo	Motherwort herb, cut	12376408	2
Caelo	Mullein flower, cut	11020714	4
Caelo	Mullein flower, cut	12170906	1
Caelo	Mullein flower, cut	11020802	2
Caelo	Mullein flower, cut	11233401	4
Caelo	Mullein flower, cut	16081201	1
Caelo	Mullein flower, cut	11020713	2
Caelo	Mullein flower, cut	521505390	1
Caelo	Mullein flower, cut	11366402	1
Caelo	Mullein flower, cut	12192903	3
Caelo	Mullein flower, cut	13229701	2
Caelo	Mullein flower, cut	12192905	5
Caelo	Mullein flower, cut	11366403	1
Caelo	Mullein flower, cut	18031301	1
Caelo	Mullein flower, cut	12317104	1
Caelo	Mullein flower, cut	12192904	1
Caelo	Mullein flower, cut	12170901	1
Caelo	Mullein flower, cut	12192907	3
Caelo	Mullein flower, cut	12192901	3
Caelo	Mullein flower, cut	11020902	1
Caelo	Mullein flower, cut	11233402	1
Caelo	Mullein flower, cut	1219203	1
Caelo	Mullein flower, cut	13229702	1
Caelo	Mullein flower, cut	11333402	1
Caelo	Myrrh	13108701	2
Caelo	Myrrh	12269907	1

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Supplier	Substance	Batch	Spectra
Caelo	Myrrh	30121413	1
Caelo	Myrrh	11277111	1
Caelo	Myrrh	11276810	1
Caelo	Myrrh	11277105	1
Caelo	Myrrh	12269913	1
Caelo	Myrrh	12244404	1
Caelo	Myrrh	28101401	1
Caelo	Myrrh	11277111	1
Caelo	Myrrh	12269904	4
Caelo	Myrrh	12244406	1
Caelo	Myrrh	12269901	2
Caelo	Myrrh	25071404	1
Caelo	Myrrh	14244602	1
Caelo	Myrrh	11276806	1
Caelo	Myrrh	15312606	1
Caelo	Nettle leaf, cut	12183911	16
Caelo	Nettle leaf, cut	12195002	2
Caelo	Nettle leaf, cut	12183908	5
Caelo	Nettle leaf, cut	120375901	1
Caelo	Nettle leaf, cut	12183909	1
Caelo	Nettle leaf, cut	intch:313011	1
Caelo	Nettle leaf, cut	83142389	1
Caelo	Nettle leaf, cut	12183901	2
Caelo	Nettle leaf, cut	13091302	1
Caelo	Nettle leaf, cut	12034402	3
Caelo	Nettle leaf, cut	2051302	1
Caelo	Nettle leaf, cut	12183910	11
Caelo	Nettle leaf, cut	14344907	1
Caelo	Nettle leaf, cut	2381A130122	22
Caelo	Nettle leaf, cut	10375901	2
Caelo	Nettle leaf, cut	12183914	8
Caelo	Nettle leaf, cut	72085497	1
Caelo	Nettle leaf, cut	10282807	2
Caelo	Nettle leaf, cut	10291405	2
Caelo	Nettle leaf, cut	7031302	1
Caelo	Nettle leaf, cut	12184004	8
Caelo	Nettle leaf, cut	12034403	8
Caelo	Nettle leaf, cut	12184001	5
Caelo	Nettle leaf, cut	12183908-3443311112	1
Caelo	Nettle leaf, cut	20111306	1
Caelo	Nettle leaf, cut	12184706	3
Caelo	Nettle leaf, cut	12183908-3391311070	1
Caelo	Nettle leaf, cut	10162712	1
Caelo	Nettle leaf, cut	1283910	1
Caelo	Nettle leaf, cut	17121205	1
Caelo	Nettle leaf, cut	18071202	1
Caelo	Nettle leaf, cut	10291411	2
Caelo	Nettle leaf, cut	12184005	7
Caelo	Nettle leaf, cut	10291414	3
Caelo	Nettle leaf, cut	29071303	1
Caelo	Nettle leaf, cut	12184702	2
Caelo	Nettle leaf, cut	12184503	3
Caelo	Nettle leaf, cut	12814001	1
Caelo	Nettle leaf, cut	12034414	1
Caelo	Nettle leaf, cut	12195101	3
Caelo	Nettle leaf, cut	12184502	2
Caelo	Nettle leaf, cut	12183908-3405310181	1
Caelo	Nettle leaf, cut	10291413	1
Caelo	Nettle leaf, cut	83374109	1
Caelo	Nettle leaf, cut		3

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Supplier	Substance	Batch	Spectra
Caelo	Nettle leaf, cut	10291422	3
Caelo	Nettle leaf, cut	33/AD1	1
Caelo	Nettle leaf, cut	10282806	1
Caelo	Nettle leaf, cut	3021401	1
Caelo	Nettle leaf, cut	13386801	1
Caelo	Nettle root, cut	6441A121024	1
Caelo	Nettle root, cut	11254903	5
Caelo	Nettle root, cut	10081202	1
Caelo	Nettle root, cut	11265003	2
Caelo	Nettle root, cut	11265002	5
Caelo	Nettle root, cut	11254904	2
Caelo	Nettle root, cut	6631B130610	1
Caelo	Nettle root, cut	11265006	1
Caelo	Nettle root, cut	11265004	4
Caelo	Nettle root, cut	11254902	3
Caelo	Nettle seed	13010612	2
Caelo	Nettle seed	13010607	1
Caelo	Nettle seed	15290602	1
Caelo	Nettle seed	12131505	1
Caelo	Nettle seed	16327001	2
Caelo	Nettle seed	20111301	1
Caelo	Nettle seed	17282601	1
Caelo	Nutmeg	12376805	1
Caelo	Nutmeg	12376802	2
Caelo	Nutmeg, powdered (spi...	12102305	2
Caelo	Oak bark, cut	13360312	5
Caelo	Oak bark, cut	3041301	1
Caelo	Oak bark, cut	11351202	5
Caelo	Oak bark, cut	13360306	1
Caelo	Oak bark, cut	14111316	1
Caelo	Oak bark, cut	13360304	1
Caelo	Oak bark, cut	41109-4-P	1
Caelo	Oak bark, cut	161212	1
Caelo	Oak bark, cut	11351210	1
Caelo	Oak bark, cut	13360302	6
Caelo	Oak bark, cut	123test	1
Caelo	Oak bark, cut	13360301	1
Caelo	Oak bark, cut	11351210	8
Caelo	Oak bark, cut	13360303	1
Caelo	Oak bark, cut	13360306	2
Caelo	Oak bark, cut	1081401	1
Caelo	Oak bark, cut	11351208	3
Caelo	Oak bark, cut	11351209	9
Caelo	Oak bark, cut	13360305	1
Caelo	Oak bark, cut	12221102	1
Caelo	Oak bark, cut	11351207-3384310110	1
Caelo	Oak bark, cut	10348615	1
Caelo	Oak bark, cut	11351205	3
Caelo	Oak bark, cut	5091302	1
Caelo	Oak bark, cut	280814A	1
Caelo	Oak bark, cut	26081302	1
Caelo	Oak bark, cut	12221104	2
Caelo	Oak bark, cut	14277004	2
Caelo	Oak bark, cut	13360311	1
Caelo	Oak bark, cut	11351207	11
Caelo	Oak bark, cut	15146104	3
Caelo	Oak bark, cut	10348605	1
Caelo	Oak bark, cut	10348613	2
Caelo	Oak bark, cut	10348612	1
Caelo	Oak bark, cut	15146109	2

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Supplier	Substance	Batch	Spectra
Caelo	Oak bark, cut	22081204	1
Caelo	Oak bark, cut	15146110	1
Caelo	Oak bark, cut	15146110	1
Caelo	Oak bark, cut	12221101	9
Caelo	Oak bark, cut	11351201	3
Caelo	Oak bark, cut	15146103	1
Caelo	Oak bark, cut	15314908	1
Caelo	Oak bark, cut	15314910	2
Caelo	Oak bark, cut	15314901	1
Caelo	Oak bark, cut	15314904	1
Caelo	Oak bark, cut	15146105	1
Caelo	Oak bark, cut	15146105	4
Caelo	Oak bark, cut	15314903	1
Caelo	Oak bark, cut	9357419	2
Caelo	Oak bark, cut	19032013	2
Caelo	Oak bark, cut	13360309	1
Caelo	Oak bark, cut	12221105	2
Caelo	Oak bark, cut	10061504	1
Caelo	Oak bark, cut	14277004	1
Caelo	Oak bark, cut	15314905	2
Caelo	Oak bark, cut	15146102	1
Caelo	Oak bark, cut	13360308	1
Caelo	Oak bark, cut	7021302	1
Caelo	Oak bark, cut	15146101	2
Caelo	Oak bark, cut	14277004	1
Caelo	Oak bark, cut	11351203	1
Caelo	Oak bark, cut	16081305	1
Caelo	Oak bark, powdered	10261513	1
Caelo	Oat straw, cut	11280014	1
Caelo	Oat straw, cut	11280015	3
Caelo	Oat straw, cut	11280017	2
Caelo	Oat straw, cut	11280008	2
Caelo	Oat straw, cut	11280012	2
Caelo	Olive leaf	12159805	1
Caelo	Oregano herb	12360901	6
Caelo	Oregano herb	11340703	2
Caelo	Oregano herb	11340709	1
Caelo	Oregano herb	12360902	2
Caelo	Oregano herb	11340705	1
Caelo	Oregano herb	12360904	1
Caelo	Oregano herb	11340708	1
Caelo	Orris root	13113401	2
Caelo	Orris root	13113402	1
Caelo	Orris root	1026706	1
Caelo	Orris root	11026704	2
Caelo	Orris root	13113404	1
Caelo	Orris root	11026706	1
Caelo	Parsley herb, rubbed	12376601	2
Caelo	Parsley herb, rubbed	51978126	1
Caelo	Parsley herb, rubbed	12376603	2
Caelo	Parsley herb, rubbed	12376602	2
Caelo	Parsley root, cut	13156005	1
Caelo	Parsley root, cut	13156003	1
Caelo	Parsley root, cut	12080304	1
Caelo	Parsley root, cut	12080309	1
Caelo	Parsley seed	PrüfNr. 2814A-01550	1
Caelo	Passionflower herb, cut	11049111	1
Caelo	Passionflower herb, cut	12031715	7
Caelo	Passionflower herb, cut	12031717	7
Caelo	Passionflower herb, cut	12031712	1

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Supplier	Substance	Batch	Spectra
Caelo	Passionflower herb, cut	12101301	1
Caelo	Passionflower herb, cut	13141201	1
Caelo	Passionflower herb, cut	13141203	2
Caelo	Passionflower herb, cut	12031701	1
Caelo	Passionflower herb, cut	12031714	2
Caelo	Passionflower herb, cut	13141205	4
Caelo	Passionflower herb, cut	15085105	1
Caelo	Passionflower herb, cut	1011A-01669	1
Caelo	Passionflower herb, cut	12031706	3
Caelo	Passionflower herb, cut	13141202	5
Caelo	Passionflower herb, cut	12031716	3
Caelo	Passionflower herb, cut	11049108	1
Caelo	Passionflower herb, cut	12031710	13
Caelo	Passionflower herb, cut	12031704	1
Caelo	Passionflower herb, cut	12031705	4
Caelo	Passionflower herb, cut	12031703	2
Caelo	Passionflower herb, cut	11049116	4
Caelo	Peppermint leaf, cut	12266908	7
Caelo	Peppermint leaf, cut	13030805	5
Caelo	Peppermint leaf, cut	Int.Ch.:313011	1
Caelo	Peppermint leaf, cut	ChB:311092	1
Caelo	Peppermint leaf, cut	13214720	1
Caelo	Peppermint leaf, cut	11347609	1
Caelo	Peppermint leaf, cut	13030804	1
Caelo	Peppermint leaf, cut	2181B090928	1
Caelo	Peppermint leaf, cut	14083102	2
Caelo	Peppermint leaf, cut	12266903	5
Caelo	Peppermint leaf, cut	1132803	1
Caelo	Peppermint leaf, cut	13030806	1
Caelo	Peppermint leaf, cut	11327801	2
Caelo	Peppermint leaf, cut	11294409	2
Caelo	Peppermint leaf, cut	20111215	1
Caelo	Peppermint leaf, cut	12054149	1
Caelo	Peppermint leaf, cut	12032311	1
Caelo	Peppermint leaf, cut	11327803	5
Caelo	Peppermint leaf, cut	20061202	1
Caelo	Peppermint leaf, cut	13105001	1
Caelo	Peppermint leaf, cut	268320	1
Caelo	Peppermint leaf, cut	13030808-3401310161	1
Caelo	Peppermint leaf, cut	11294401	3
Caelo	Peppermint leaf, cut	12032319	2
Caelo	Peppermint leaf, cut	14339202	2
Caelo	Peppermint leaf, cut	12266913	9
Caelo	Peppermint leaf, cut	12266912	1
Caelo	Peppermint leaf, cut	6011403	1
Caelo	Peppermint leaf, cut	5091307	1
Caelo	Peppermint leaf, cut	2181A1209-13	1
Caelo	Peppermint leaf, cut	13214707	2
Caelo	Peppermint leaf, cut	13214706	1
Caelo	Peppermint leaf, cut	13030809	2
Caelo	Peppermint leaf, cut	14221701	1
Caelo	Peppermint leaf, cut	13030807	3
Caelo	Peppermint leaf, cut	12266904	2
Caelo	Peppermint leaf, cut	8101301	1
Caelo	Peppermint leaf, cut	13030808	1
Caelo	Peppermint leaf, cut	161212	1
Caelo	Peppermint leaf, cut	13214705	1
Caelo	Phenol	11163809	1
Caelo	Phenol	11163801	1
Caelo	Phenol	12223001	1

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Supplier	Substance	Batch	Spectra
Caelo	Phenol	11163802	1
Caelo	Phenol	7061305	1
Caelo	Phenol	12223014	1
Caelo	Phenol	12223020	1
Caelo	Phenol	12223022	1
Caelo	Piper cubeba	11081903	1
Caelo	Podophyllum resin (fr...	11085811	1
Caelo	Podophyllum resin (fr...	12379903	1
Caelo	Podophyllum resin (fr...	11085807	4
Caelo	Podophyllum resin (fr...	12287805	1
Caelo	Podophyllum resin (fr...	82433349	1
Caelo	Podophyllum resin (fr...	12287810	1
Caelo	Potassium hydrocarbon...	20080410-3	1
Caelo	Potassium hydrocarbon...	10052622	1
Caelo	Potassium hydrocarbon...	12141924	3
Caelo	Potassium hydrocarbon...	10052610	1
Caelo	Potassium hydrocarbon...	11105822	1
Caelo	Potassium hydrocarbon...	11105811	3
Caelo	Potassium hydrocarbon...	12141905	3
Caelo	Potassium hydrocarbon...	1011M-01728	1
Caelo	Potassium hydrocarbon...	8101202	1
Caelo	Potassium hydrocarbon...	12239702	2
Caelo	Potassium hydrocarbon...	11105818	1
Caelo	Potassium hydrocarbon...	11105804	1
Caelo	Potassium hydrocarbon...	11105812	1
Caelo	Potassium hydrocarbon...	11105808	1
Caelo	Potassium hydrocarbon...	12239701	3
Caelo	Potassium hydrocarbon...	12239703	3
Caelo	Potassium hydrocarbon...	6011405	1
Caelo	Potassium hydrocarbon...	IntCh:217002	1
Caelo	Potassium hydrocarbon...	3812Q-01728	1
Caelo	Potassium hydrocarbon...	700544	1
Caelo	Potassium hydrocarbon...	1214190	1
Caelo	Potassium hydrocarbon...	12141920	1
Caelo	Potassium hydrocarbon...	1214924	1
Caelo	Potassium hydrocarbon...	1303002-01	5
Caelo	Potassium hydrocarbon...	12141912	2
Caelo	Potassium hydrocarbon...	13141926	1
Caelo	Potassium hydrocarbon...	12141915	4
Caelo	Potassium hydrocarbon...	12141919	3
Caelo	Potassium hydrocarbon...	10052629	1
Caelo	Potassium hydrocarbon...	13390307	1
Caelo	Potassium hydrocarbon...	12141930	2
Caelo	Potassium hydrocarbon...	12141910	8
Caelo	Potassium hydrocarbon...	13390303	1
Caelo	Potassium hydrocarbon...	24051301	1
Caelo	Potassium hydroxide	12057912	2
Caelo	Potassium hydroxide	12382603	4
Caelo	Potassium hydroxide	12382606	2
Caelo	Potassium hydroxide	12057906	1
Caelo	Potassium hydroxide	12382601	2
Caelo	Potassium hydroxide	11165705	1
Caelo	Potassium hydroxide	12382611	1
Caelo	Potassium hydroxide	11165708	1
Caelo	Potassium hydroxide	17091202	1
Caelo	Potassium hydroxide	12057908	2
Caelo	Potassium hydroxide	12057905	1
Caelo	Potassium hydroxide	27111310	1
Caelo	Potassium hydroxide	13275207	1
Caelo	Potassium hydroxide	13275201	1

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Supplier	Substance	Batch	Spectra
Caelo	Primrose flower	10207104	1
Caelo	Primrose flower	11206807	1
Caelo	Primrose flower	5021303	1
Caelo	Primrose flower	11374403	1
Caelo	Primrose flower	113744044	1
Caelo	Primrose flower	25091306	1
Caelo	Primrose flower	9021301	1
Caelo	Primrose flower	11206808	1
Caelo	Primrose flower	11206811	4
Caelo	Primrose flower	11206810	5
Caelo	Primrose flower	11374404	1
Caelo	Primrose flower	13086603	5
Caelo	Primrose flower	11374401	10
Caelo	Primrose flower	1308660	1
Caelo	Primrose flower	11206811	1
Caelo	Primrose flower	11206803	4
Caelo	Primrose flower	13086602	5
Caelo	Primrose flower	13086602	2
Caelo	Primrose flower	13086603	1
Caelo	Primrose flower	10072509	1
Caelo	Primrose flower	13086605	1
Caelo	Primrose flower	11374402	1
Caelo	Primrose flower	13276904	1
Caelo	Primrose flower	13086608	1
Caelo	Primrose flower	11206804	1
Caelo	Primrose flower	11374403	3
Caelo	Primrose root, cut	13087004	1
Caelo	Primrose root, cut	12064506	4
Caelo	Primrose root, cut	13087005-3534411072	1
Caelo	Primrose root, cut	10382012	1
Caelo	Primrose root, cut	13087002	4
Caelo	Primrose root, cut	10382010	1
Caelo	Primrose root, cut	24011301	1
Caelo	Primrose root, cut	Int.Ch:318090	1
Caelo	Primrose root, cut	10382009	1
Caelo	Primrose root, cut	13087005	3
Caelo	Primrose root, cut	13067001	1
Caelo	Primrose root, cut	5010E-02159	1
Caelo	Primrose root, cut	10382013	1
Caelo	Primrose root, cut	71653517	1
Caelo	Primrose root, cut	4021410	1
Caelo	Primrose root, cut	13087001	1
Caelo	Primrose root, cut	12064503	1
Caelo	Psyllium seed	13305910	4
Caelo	Psyllium seed	13305906	2
Caelo	Psyllium seed	13305903	1
Caelo	Psyllium seed	13305904	2
Caelo	Psyllium seed	12140301	7
Caelo	Psyllium seed	13234309	1
Caelo	Psyllium seed	7380a120911	1
Caelo	Psyllium seed	10291207	6
Caelo	Psyllium seed	12276510	1
Caelo	Psyllium seed	12185502	1
Caelo	Psyllium seed	12185508	3
Caelo	Psyllium seed	12185509	5
Caelo	Psyllium seed	10291204	1
Caelo	Psyllium seed	12185503	3
Caelo	Psyllium seed	11185803	1
Caelo	Psyllium seed	12185504	10
Caelo	Psyllium seed	11185811	4

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Supplier	Substance	Batch	Spectra
Caelo	Psyllium seed	10291205	1
Caelo	Psyllium seed	13234310	3
Caelo	Psyllium seed	13305907	5
Caelo	Psyllium seed	10061503	1
Caelo	Psyllium seed	10291206	1
Caelo	Psyllium seed	15190303	4
Caelo	Psyllium seed	15190304	3
Caelo	Psyllium seed	15190306	1
Caelo	Pumpkin seed, peeled	140736306	1
Caelo	Pumpkin seed, peeled	122490911	1
Caelo	Pumpkin seed, peeled	16081206	2
Caelo	Pumpkin seed, peeled	12249001	2
Caelo	Pumpkin seed, peeled	12249011	2
Caelo	Pumpkin seed, peeled	14073603	1
Caelo	Pumpkin seed, peeled	16081202	1
Caelo	Pumpkin seed, peeled	14186910	1
Caelo	Pumpkin seed, peeled	14186905	1
Caelo	Ramsons herb, cut	11182207	1
Caelo	Ramsons herb, cut	11182204	1
Caelo	Ramsons herb, cut	11182203	1
Caelo	Ramsons herb, cut	12380803	1
Caelo	Ramsons herb, cut	14343305	1
Caelo	Ramsons herb, cut	12380801	2
Caelo	Ramsons herb, cut	12380802	2
Caelo	Raspberry leaf, cut	11030706	3
Caelo	Raspberry leaf, cut	713E-01511	1
Caelo	Raspberry leaf, cut	13038002	1
Caelo	Raspberry leaf, cut	12362706	29
Caelo	Raspberry leaf, cut	17121203	1
Caelo	Raspberry leaf, cut	13127901	3
Caelo	Raspberry leaf, cut	1210315	1
Caelo	Raspberry leaf, cut	12392709	1
Caelo	Raspberry leaf, cut	1310603	1
Caelo	Raspberry leaf, cut	30011408	1
Caelo	Raspberry leaf, cut	13101605	1
Caelo	Raspberry leaf, cut	25091201	1
Caelo	Raspberry leaf, cut	6859427	1
Caelo	Raspberry leaf, cut	12103109	2
Caelo	Raspberry leaf, cut	10136412	1
Caelo	Raspberry leaf, cut	2909211511	1
Caelo	Raspberry leaf, cut	11121201	1
Caelo	Raspberry leaf, cut	12103108	8
Caelo	Raspberry leaf, cut	11030707	3
Caelo	Raspberry leaf, cut	10136404	1
Caelo	Raspberry leaf, cut	14018803	1
Caelo	Raspberry leaf, cut	18101203	1
Caelo	Raspberry leaf, cut	12362710	13
Caelo	Raspberry leaf, cut	9101204	1
Caelo	Raspberry leaf, cut	21051302	1
Caelo	Raspberry leaf, cut	9011404	1
Caelo	Raspberry leaf, cut	2271C120508	5
Caelo	Raspberry leaf, cut	12368706	1
Caelo	Raspberry leaf, cut	11030705	1
Caelo	Raspberry leaf, cut	11071301	1
Caelo	Raspberry leaf, cut	18041304	1
Caelo	Raspberry leaf, cut	13038003	1
Caelo	Raspberry leaf, cut	13101602-347312141	1
Caelo	Raspberry leaf, cut	13101803	1
Caelo	Raspberry leaf, cut	231013c	1
Caelo	Raspberry leaf, cut	12362709	5

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Supplier	Substance	Batch	Spectra
Caelo	Raspberry leaf, cut	13101604	3
Caelo	Raspberry leaf, cut	7011402	1
Caelo	Raspberry leaf, cut	IntCh:311090	1
Caelo	Raspberry leaf, cut	1236705	1
Caelo	Raspberry leaf, cut	12362710-3432311160	1
Caelo	Raspberry leaf, cut	11030704	2
Caelo	Raspberry leaf, cut	10013410	1
Caelo	Raspberry leaf, cut	12362704	5
Caelo	Raspberry leaf, cut	12362708	3
Caelo	Raspberry leaf, cut	22081201	1
Caelo	Raspberry leaf, cut	9081205	1
Caelo	Raspberry leaf, cut	12103101	7
Caelo	Raspberry leaf, cut	12362707	4
Caelo	Raspberry leaf, cut	12103111	15
Caelo	Raspberry leaf, cut	20081311	1
Caelo	Raspberry leaf, cut	10013411	1
Caelo	Raspberry leaf, cut	12130107	1
Caelo	Raspberry leaf, cut	12362711	9
Caelo	Raspberry leaf, cut	307211511	1
Caelo	Raspberry leaf, cut	13101603	5
Caelo	Raspberry leaf, cut	12362702	7
Caelo	Raspberry leaf, cut	10013409	2
Caelo	Raspberry leaf, cut	12362705	9
Caelo	Raspberry leaf, cut	8031307	1
Caelo	Raspberry leaf, cut	10013407	1
Caelo	Raspberry leaf, cut	314U1511	1
Caelo	Red poppy petals, cut	12330205	1
Caelo	Red-rose petal	12380004	1
Caelo	Red-rose petal	12380008	2
Caelo	Red-rose petal, cut	12380007-3357319071	1
Caelo	Red-rose petal, cut	12380008	1
Caelo	Red-rose petal, cut	10113211	1
Caelo	Red-rose petal, cut	12380004	2
Caelo	Red-rose petal, cut	11304912	2
Caelo	Red-rose petal, cut	13194403	4
Caelo	Red-rose petal, cut	13194402	1
Caelo	Red-rose petal, cut	11011301	1
Caelo	Red-rose petal, cut	11304904	4
Caelo	Red-rose petal, cut	12380001	4
Caelo	Red-rose petal, cut	11304901	3
Caelo	Red-rose petal, cut	10306514	1
Caelo	Red-rose petal, cut	11304906	1
Caelo	Redwood	12049608	2
Caelo	Redwood	12049607	2
Caelo	Redwood	13106901	1
Caelo	Redwood	12041403	1
Caelo	Restharrow root, cut	11103107	2
Caelo	Restharrow root, cut	11103105	2
Caelo	Restharrow root, cut	6101201	1
Caelo	Restharrow root, cut	11247302	2
Caelo	Restharrow root, cut	12300004	1
Caelo	Restharrow root, cut	4021406	1
Caelo	Restharrow root, cut	71035467	1
Caelo	Restharrow root, cut	Int.Ch:212150	1
Caelo	Restharrow root, cut	21011306	1
Caelo	Restharrow root, cut	12330005	5
Caelo	Restharrow root, cut	12330001	11
Caelo	Restharrow root, cut	12330003	2
Caelo	Restharrow root, cut	12330002	1
Caelo	Restharrow root, cut	1233001	1

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Supplier	Substance	Batch	Spectra
Caelo	Restharrow root, cut	72439069	1
Caelo	Restharrow root, cut	20111213	1
Caelo	Restharrow root, cut	15101313	1
Caelo	Rhubarb, cut	11321806	1
Caelo	Rhubarb, cut	11265902	1
Caelo	Rhubarb, cut	11057818	2
Caelo	Rhubarb, cut	12211903	4
Caelo	Rhubarb, cut	12211902	3
Caelo	Rhubarb, cut	11057810	1
Caelo	Rhubarb, cut	12211904	2
Caelo	Rhubarb, cut	12211906	1
Caelo	Rhubarb, cut	11057804	1
Caelo	Rhubarb, cut	10071302	1
Caelo	Rhubarb, cut	12211908	1
Caelo	Rhubarb, cut	13235205	1
Caelo	Rhubarb, cut	25111305	1
Caelo	Rhubarb, cut	13235203	1
Caelo	Rhubarb, cut	13235201	2
Caelo	Rhubarb, cut	15101301	1
Caelo	Rhubarb, cut	14155404	1
Caelo	Rhubarb, powdered	13193104	4
Caelo	Rhubarb, powdered	23061402	1
Caelo	Rhubarb, powdered	13193109	1
Caelo	Rhubarb, powdered	11043826	1
Caelo	Rhubarb, powdered	11043816	1
Caelo	Rhubarb, powdered	13193106	2
Caelo	Rhubarb, powdered	11043822	1
Caelo	Rhubarb, powdered	11043818	1
Caelo	Rhubarb, powdered	11043819	2
Caelo	Rhubarb, powdered	11043818	1
Caelo	Rhubarb, powdered	11043817	1
Caelo	Rhubarb, powdered	11043816	2
Caelo	Rhubarb, powdered	11043825	2
Caelo	Rhubarb, powdered	9071201	1
Caelo	Ribwort plantain, cut	1313007	1
Caelo	Ribwort plantain, cut	13410603	3
Caelo	Ribwort plantain, cut	13410601	1
Caelo	Ribwort plantain, cut	15096308	1
Caelo	Ribwort plantain, cut	14199202	1
Caelo	Ribwort plantain, cut	15096301	1
Caelo	Ribwort plantain, cut	13113001	7
Caelo	Ribwort plantain, cut	13410612	1
Caelo	Ribwort plantain, cut	4021411	1
Caelo	Ribwort plantain, cut	25041301	1
Caelo	Ribwort plantain, cut	10328702	2
Caelo	Ribwort plantain, cut	13113008	5
Caelo	Ribwort plantain, cut	13113007	6
Caelo	Ribwort plantain, cut	20111304	1
Caelo	Ribwort plantain, cut	15111302	1
Caelo	Ribwort plantain, cut	22021302	1
Caelo	Ribwort plantain, cut	13113005	5
Caelo	Ribwort plantain, cut	10315705	1
Caelo	Ribwort plantain, cut	13113006	5
Caelo	Ribwort plantain, cut	23121304	1
Caelo	Ribwort plantain, cut	2031302	1
Caelo	Ribwort plantain, cut	12362903-3388311070	1
Caelo	Ribwort plantain, cut	1362903	1
Caelo	Ribwort plantain, cut	12362901	1
Caelo	Ribwort plantain, cut	25091305	1
Caelo	Ribwort plantain, cut	12362906	7

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Supplier	Substance	Batch	Spectra
Caelo	Ribwort plantain, cut	28061301	1
Caelo	Ribwort plantain, cut	11061304	1
Caelo	Ribwort plantain, cut	31051316	1
Caelo	Ribwort plantain, cut	16101304	1
Caelo	Ribwort plantain, cut	13113004-3488312172	1
Caelo	Ribwort plantain, cut	17071201	1
Caelo	Ribwort plantain, cut	10011402	1
Caelo	Ribwort plantain, cut	19121202	1
Caelo	Ribwort plantain, cut	10315714	2
Caelo	Ribwort plantain, cut	12225804	1
Caelo	Ribwort plantain, cut	10315711	4
Caelo	Ribwort plantain, cut	12225803	2
Caelo	Ribwort plantain, cut	15101204	1
Caelo	Ribwort plantain, cut	12225802	5
Caelo	Ribwort plantain, cut	20111208	1
Caelo	Ribwort plantain, cut	13232401	1
Caelo	Ribwort plantain, cut	13113010	4
Caelo	Ribwort plantain, cut	12362902	7
Caelo	Ribwort plantain, cut	10315715	8
Caelo	Ribwort plantain, cut	8061208	1
Caelo	Ribwort plantain, cut	10315707	2
Caelo	Ribwort plantain, cut	10315712	2
Caelo	Robert herb, cut	8121203	1
Caelo	Robert herb, cut	11147807	3
Caelo	Robert herb, cut	11147813	2
Caelo	Robert herb, cut	12319304	2
Caelo	Robert herb, cut	12319305	1
Caelo	Robert herb, cut	11147812	3
Caelo	Robert herb, cut	12319302	1
Caelo	Robert herb, cut	11147804	1
Caelo	Rose hips peel, cut	13317805	1
Caelo	Rose hips peel, cut	11301405	2
Caelo	Rose hips peel, cut	25061203	1
Caelo	Rose hips peel, cut	10101206	1
Caelo	Rose hips peel, cut	11301407	12
Caelo	Rose hips peel, cut	11301401	1
Caelo	Rose hips peel, cut	15061210	1
Caelo	Rose hips peel, cut	12288302	5
Caelo	Rose hips peel, cut	12064207	1
Caelo	Rose hips peel, cut	7031305	1
Caelo	Rose hips peel, cut	12288301	1
Caelo	Rose hips peel, cut	12357501	1
Caelo	Rose hips peel, cut	12357502	2
Caelo	Rose hips peel, cut	11301403	2
Caelo	Rose hips peel, cut	12357505	6
Caelo	Rose hips peel, cut	2851A120904konv.	1
Caelo	Rose hips peel, cut	5091301	1
Caelo	Rose hips peel, cut	12357504	2
Caelo	Rose hips peel, cut	14050705	1
Caelo	Rose hips peel, cut	14050704	1
Caelo	Rose hips peel, cut	13317801	2
Caelo	Rose hips peel, cut	9121301	1
Caelo	Rose hips peel, cut	10157309	1
Caelo	Rose hips with peel, ...	16111201	1
Caelo	Rose hips with peel, ...	13048703	1
Caelo	Rose hips with peel, ...	12064202	1
Caelo	Rose hips with peel, ...	12064202	1
Caelo	Rose hips with peel, ...	19111204	1
Caelo	Rose hips with peel, ...	12064207	2
Caelo	Rose hips with peel, ...	12064206	1

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Supplier	Substance	Batch	Spectra
Caelo	Rose hips with peel, ...	1512211542	1
Caelo	Rose hips with peel, ...	12064207	3
Caelo	Rose hips with peel, ...	12064210	3
Caelo	Rose hips with peel, ...	2103311542	1
Caelo	Rose hips with peel, ...	12064201	1
Caelo	Rose hips with peel, ...	12064212	3
Caelo	Rose hips with peel, ...	307211542	1
Caelo	Rose hips with peel, ...	12064210	1
Caelo	Rose hips with peel, ...	12064212	2
Caelo	Rose hips with peel, ...	12064209	4
Caelo	Rose hips with peel, ...	12029011	1
Caelo	Rose hips with peel, ...	12064213	1
Caelo	Rose hips with peel, ...	12064213	1
Caelo	Rose hips with peel, ...	12029008	1
Caelo	Rose hips with peel, ...	13097405	1
Caelo	Rose hips with peel, ...	13048703	1
Caelo	Rose hips with peel, ...	13048701	2
Caelo	Rose hips with peel, ...	13048704	1
Caelo	Rose hips with peel, ...	13048704	3
Caelo	Rose hips with peel, ...	12064209	1
Caelo	Rose hips with peel, ...	114Q-01542	1
Caelo	Rose mallow flower, cut	13040401	2
Caelo	Rose mallow flower, cut	13040402	1
Caelo	Rose mallow flower, cut	10244507	1
Caelo	Roselle	12267504-3428311150	1
Caelo	Roselle	7121301	1
Caelo	Roselle	11036512	1
Caelo	Roselle	12267503	2
Caelo	Roselle	12267504	1
Caelo	Roselle	11036509	1
Caelo	Roselle	11036511	1
Caelo	Roselle	12267502	4
Caelo	Roselle	12267507	2
Caelo	Roselle	12267504	3
Caelo	Roselle	12007306	1
Caelo	Roselle	12267502	3
Caelo	Roselle	11036504	1
Caelo	Roselle	12267501	3
Caelo	Rosemary leaf, cut	13128805	1
Caelo	Rosemary leaf, cut	15125008	1
Caelo	Rosemary leaf, cut	14159601	1
Caelo	Rosemary leaf, cut	1415901	1
Caelo	Rosemary leaf, cut	15125001	2
Caelo	Rosemary leaf, cut	17352502	1
Caelo	Rosemary leaf, cut	28051404	1
Caelo	Rosemary leaf, cut	14082901	1
Caelo	Rosemary leaf, cut	13128801	1
Caelo	Rosemary leaf, cut	13128802	2
Caelo	Rosemary leaf, cut	12225902	1
Caelo	Rosemary leaf, cut	IntCh:313060	1
Caelo	Rosemary leaf, cut	11193406	1
Caelo	Rosemary leaf, cut	5041302	1
Caelo	Rosemary leaf, cut	11193408	6
Caelo	Rosemary leaf, cut	11193404	1
Caelo	Rosemary leaf, cut	11193405	1
Caelo	Rosemary leaf, cut	11193405	1
Caelo	Rosemary leaf, cut	11193402	2
Caelo	Rosemary leaf, cut	13128806	2
Caelo	Rue herb, cut	12148801	1
Caelo	Rue herb, cut	11371803	1

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Supplier	Substance	Batch	Spectra
Caelo	Rue herb, cut	12148806	1
Caelo	Rue herb, cut	12148804	1
Caelo	Rue herb, cut	12148803	2
Caelo	Rue herb, cut	9336802	1
Caelo	Rue herb, cut		1
Caelo	Saffron filaments	11071310	1
Caelo	Saffron filaments	21011403	1
Caelo	Saffron filaments	12108311	2
Caelo	Saffron filaments	15101305	1
Caelo	Saffron filaments	12108308	2
Caelo	Saffron filaments	10184822	1
Caelo	Saffron filaments	10184811	2
Caelo	Sage leaf, cut	15041304	1
Caelo	Sage leaf, cut	22081203	1
Caelo	Sage leaf, cut	31081202	1
Caelo	Sage leaf, cut	11056123	5
Caelo	Sage leaf, cut	1209211513	1
Caelo	Sage leaf, cut	279939	1
Caelo	Sage leaf, cut	123770010	1
Caelo	Sage leaf, cut	410211513	1
Caelo	Sage leaf, cut	14111315	1
Caelo	Sage leaf, cut	22061201	1
Caelo	Sage leaf, cut	9121302	1
Caelo	Sage leaf, cut	12370014-3477312161	1
Caelo	Sage leaf, cut	12370015	2
Caelo	Sage leaf, cut	8011420	1
Caelo	Sage leaf, cut	12380009	1
Caelo	Sage leaf, cut	13011405	1
Caelo	Sage leaf, cut	12370017	1
Caelo	Sage leaf, cut	12370014-3541411092	1
Caelo	Sage leaf, cut	13266603	2
Caelo	Sage leaf, cut	13266605	3
Caelo	Sage leaf, cut	13266606	1
Caelo	Sage leaf, cut	13266621	1
Caelo	Sage leaf, cut	13266626	1
Caelo	Sage leaf, cut	11056109	5
Caelo	Sage leaf, cut	111012004	1
Caelo	Sage leaf, cut	12370014	8
Caelo	Sage leaf, cut	15121201	1
Caelo	Sage leaf, cut	12370006	8
Caelo	Sage leaf, cut	12370009	12
Caelo	Sage leaf, cut	12370001	16
Caelo	Sage leaf, cut	103311513	1
Caelo	Sage leaf, cut	12021302	1
Caelo	Sage leaf, cut	11347509	4
Caelo	Sage leaf, cut	11347511	9
Caelo	Sage leaf, cut	20121201	1
Caelo	Sage leaf, cut	12370011	11
Caelo	Sage leaf, cut	12370004	2
Caelo	Sage leaf, cut	12370003	4
Caelo	Sage leaf, cut	22111203	1
Caelo	Sage leaf, cut	17061302	1
Caelo	Sage leaf, cut	12112101	1
Caelo	Sage leaf, cut	11347508	3
Caelo	Sage leaf, cut	25061302	1
Caelo	Sage leaf, cut	312010	1
Caelo	Sage leaf, cut	26081301	1
Caelo	Sage leaf, cut	12370003-3359319071	1
Caelo	Sage leaf, cut	11347503	1
Caelo	Sage leaf, cut	11056125	3

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Supplier	Substance	Batch	Spectra
Caelo	Sage leaf, cut	12370013	3
Caelo	Sage leaf, cut	1237003	1
Caelo	Sage leaf, cut	11347513	1
Caelo	Sarsaparilla root, cut	13079201	1
Caelo	Savory, rubbed	12177207	1
Caelo	Savory, rubbed	12200801	1
Caelo	Savory, rubbed	13172404	2
Caelo	Savory, rubbed	12177201	1
Caelo	Savory, rubbed	12177203	7
Caelo	Senna leaf, cut	131316701	1
Caelo	Senna leaf, cut	12115502	1
Caelo	Senna leaf, cut	12273119	4
Caelo	Senna leaf, cut	11277305	1
Caelo	Senna leaf, cut	2231B13014	1
Caelo	Senna leaf, cut	12273113	3
Caelo	Senna leaf, cut	12273114	2
Caelo	Senna leaf, cut	11041009	1
Caelo	Senna leaf, cut	1803311514	1
Caelo	Senna leaf, cut	12273105	6
Caelo	Senna leaf, cut	12273101	3
Caelo	Senna leaf, cut	12273115	11
Caelo	Senna leaf, cut	103311514	2
Caelo	Senna leaf, cut	12273111	10
Caelo	Senna leaf, cut	9071302	1
Caelo	Senna leaf, cut	12273107	9
Caelo	Senna leaf, cut	12273106	3
Caelo	Senna leaf, cut	1273103	1
Caelo	Senna leaf, cut	2331B120521	4
Caelo	Senna leaf, cut	711211514	1
Caelo	Senna leaf, cut	10126502	1
Caelo	Senna leaf, cut	12115503	6
Caelo	Senna leaf, cut	2909211514	1
Caelo	Senna leaf, cut	12115501	5
Caelo	Senna leaf, cut	11277301	1
Caelo	Senna leaf, cut	18071201	1
Caelo	Senna leaf, cut	11277304	4
Caelo	Senna leaf, cut	11277307	1
Caelo	Senna leaf, cut	806211514	1
Caelo	Senna leaf, cut	12273104	2
Caelo	Senna leaf, cut	12273120	3
Caelo	Senna leaf, cut	2413Q01514	1
Caelo	Senna leaf, cut	14306324	1
Caelo	Senna leaf, cut	5013U01514	1
Caelo	Senna leaf, cut	13136705-3489312103	1
Caelo	Senna leaf, cut	13136706	1
Caelo	Senna leaf, cut	21011401	1
Caelo	Senna leaf, cut	514R1514	1
Caelo	Senna leaf, cut	1316706	1
Caelo	Senna leaf, cut	12369903	1
Caelo	Senna leaf, cut	13136718	1
Caelo	Senna leaf, cut	13136724	1
Caelo	Senna leaf, cut	14183805	2
Caelo	Senna leaf, cut	14306310	1
Caelo	Senna leaf, cut	14306311	2
Caelo	Senna leaf, cut	12276111	1
Caelo	Senna leaf, cut	111113a	1
Caelo	Senna leaf, cut	13136705	3
Caelo	Senna leaf, cut	11277316	4
Caelo	Senna leaf, cut	13136703	3
Caelo	Senna leaf, cut	15101303	1

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Supplier	Substance	Batch	Spectra
Caelo	Senna leaf, cut	12273118	3
Caelo	Senna leaf, cut	313082	1
Caelo	Senna leaf, cut	4113Q1514	1
Caelo	Senna leaf, cut	5091306	1
Caelo	Senna leaf, cut	3813E1514	1
Caelo	Senna leaf, cut	1316703	2
Caelo	Senna leaf, cut	13136704	13
Caelo	Senna leaf, powdered	11193307	1
Caelo	Senna leaf, powdered	14347606	1
Caelo	Senna pods, tinnevelly	11003009	2
Caelo	Senna pods, tinnevelly	11003004	1
Caelo	Senna pods, tinnevelly	12267608	1
Caelo	Senna pods, tinnevelly	122676707	1
Caelo	Senna pods, tinnevelly	12267606	1
Caelo	Senna pods, tinnevelly	12267605	1
Caelo	Senna pods, tinnevelly	12267201	1
Caelo	Senna pods, tinnevelly	12267602	2
Caelo	Senna pods, tinnevelly	12267604	1
Caelo	Senna pods, tinnevelly	12267609	3
Caelo	Senna pods, tinnevelly	22061202	1
Caelo	Senna pods, tinnevelly	12267610	1
Caelo	Senna pods, tinnevelly	12267007	1
Caelo	Senna pods, tinnevelly	11003013	1
Caelo	Senna pods, tinnevelly	110030009	1
Caelo	Shepherd's purse, cut	12354203	10
Caelo	Shepherd's purse, cut	12354204	16
Caelo	Shepherd's purse, cut	15101202	1
Caelo	Shepherd's purse, cut	11328203	5
Caelo	Shepherd's purse, cut	1132820111-14	1
Caelo	Shepherd's purse, cut	11091202	1
Caelo	Shepherd's purse, cut	11328201	6
Caelo	Shepherd's purse, cut	11036410	2
Caelo	Shepherd's purse, cut	14061201	1
Caelo	Shepherd's purse, cut	11036401	1
Caelo	Shepherd's purse, cut	11036406	5
Caelo	Shepherd's purse, cut	11036404	1
Caelo	Shepherd's purse, cut	12354503	1
Caelo	Shepherd's purse, cut	3121301	1
Caelo	Shepherd's purse, cut	12254202	1
Caelo	Shepherd's purse, cut	13344203	1
Caelo	Shepherd's purse, cut	12354209	1
Caelo	Shepherd's purse, cut	12354207	2
Caelo	Shepherd's purse, cut	11328207	8
Caelo	Shepherd's purse, cut	12354206	4
Caelo	Shepherd's purse, cut	11328208	6
Caelo	Shepherd's purse, cut	11328204	3
Caelo	Shepherd's purse, cut	12354202	2
Caelo	Shepherd's purse, cut	11328206	2
Caelo	Shepherd's purse, cut	10061301	1
Caelo	Shepherd's purse, cut	11328205	1
Caelo	Shepherd's purse, cut	12354205	6
Caelo	Shepherd's purse, cut	12354201	11
Caelo	Shepherd's purse, cut	11328209	6
Caelo	Shepherd's purse, cut	12354203-3396310111	1
Caelo	Silverweed, cut	11016404	1
Caelo	Silverweed, cut	20081202	1
Caelo	Silverweed, cut	8111204	1
Caelo	Silverweed, cut	11328105	7
Caelo	Silverweed, cut	11016407	1
Caelo	Silverweed, cut	11328109	13

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Supplier	Substance	Batch	Spectra
Caelo	Silverweed, cut	11328110	1
Caelo	Silverweed, cut	11328112	2
Caelo	Sodium carbonate deca...	12239810	2
Caelo	Sodium carbonate deca...	11254706	1
Caelo	Sodium carbonate deca...	13036909	1
Caelo	Sodium carbonate deca...	13036902	2
Caelo	Sodium carbonate deca...	80136428	1
Caelo	Sodium carbonate deca...	13036907	1
Caelo	Sodium carbonate deca...	13036910	1
Caelo	Sodium carbonate deca...	11254708	1
Caelo	Sodium carbonate deca...	80136179	1
Caelo	Sodium carbonate deca...	12239806	1
Caelo	Sodium dihydrogen pho...	12198506	1
Caelo	Sodium dihydrogen pho...	13D08-N25	1
Caelo	Sodium dihydrogen pho...	12198517	2
Caelo	Sodium dihydrogen pho...	12198510	2
Caelo	Sodium hydrogen carbo...	15328602	1
Caelo	Sodium hydrogen carbo...	13101706	1
Caelo	Sodium hydrogen carbo...	13234005	4
Caelo	Sodium hydrogen carbo...	13234205	1
Caelo	Sodium hydrogen carbo...	12109205	6
Caelo	Sodium hydrogen carbo...	13186711	1
Caelo	Sodium hydrogen carbo...	13390520	1
Caelo	Sodium hydrogen carbo...	13186706	1
Caelo	Sodium hydrogen carbo...	11304813	1
Caelo	Sodium hydrogen carbo...	12132204	7
Caelo	Sodium hydrogen carbo...	12132503	1
Caelo	Sodium hydrogen carbo...	13234007	4
Caelo	Sodium hydrogen carbo...	13060120	5
Caelo	Sodium hydrogen carbo...	1234702	2
Caelo	Sodium hydrogen carbo...	12324708	1
Caelo	Sodium hydrogen carbo...	12356401	3
Caelo	Sodium hydrogen carbo...	1203030-1	1
Caelo	Sodium hydrogen carbo...	11304802	2
Caelo	Sodium hydrogen carbo...	3012Q-01892	1
Caelo	Sodium hydrogen carbo...	1219204	1
Caelo	Sodium hydrogen carbo...	13060117	1
Caelo	Sodium hydrogen carbo...	13186704	1
Caelo	Sodium hydrogen carbo...	13186721	1
Caelo	Sodium hydrogen carbo...	12324725	1
Caelo	Sodium hydrogen carbo...	12324702	7
Caelo	Sodium hydrogen carbo...	13060103	8
Caelo	Sodium hydrogen carbo...	13234202	3
Caelo	Sodium hydrogen carbo...	12356303	3
Caelo	Sodium hydrogen carbo...	11304809	1
Caelo	Sodium hydrogen carbo...	12132219	8
Caelo	Sodium hydrogen carbo...	13234004	2
Caelo	Sodium hydrogen carbo...	8101203	1
Caelo	Sodium hydrogen carbo...	12356407	2
Caelo	Sodium hydrogen carbo...	12109204	3
Caelo	Sodium hydrogen carbo...	6011404	1
Caelo	Sodium hydrogen carbo...	13390505	1
Caelo	Sodium hydrogen carbo...	12356403	1
Caelo	Sodium hydrogen carbo...	12132203	3
Caelo	Sodium hydroxide pell...	11070821	1
Caelo	Sodium hydroxide pell...	15312102	1
Caelo	Sodium hydroxide pell...	12368105	1
Caelo	Sodium monohydrogenph...	12345016	7
Caelo	Sodium monohydrogenph...	12345007	3
Caelo	Sodium monohydrogenph...	9302613	2

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Supplier	Substance	Batch	Spectra
Caelo	Sodium monohydrogenph...	12345025	1
Caelo	Sodium monohydrogenph...	71199028	1
Caelo	Sodium monohydrogenph...	83002059	1
Caelo	Sodium monohydrogenph...	11169303	2
Caelo	Sodium monohydrogenph...	AKD7	1
Caelo	Sodium monohydrogenph...	11169315	1
Caelo	Sodium monohydrogenph...	12345013	6
Caelo	Sodium monohydrogenph...	1169315	1
Caelo	Sodium monohydrogenph...	12256602	2
Caelo	Sodium monohydrogenph...	12345001	2
Caelo	Sodium monohydrogenph...	12345004	7
Caelo	Sodium monohydrogenph...	11169309	3
Caelo	Sodium monohydrogenph...	13028103	1
Caelo	Sodium monohydrogenph...	12109109	1
Caelo	Sodium monohydrogenph...	12109002	2
Caelo	Sodium monohydrogenph...	10135304	1
Caelo	Sodium monohydrogenph...	11109513	1
Caelo	Sodium monohydrogenph...	13028001	1
Caelo	Sodium monohydrogenph...	72006059	1
Caelo	Sodium monohydrogenph...	12109106	1
Caelo	Sodium monohydrogenph...	13028003	1
Caelo	Sodium monohydrogenph...	12109108	2
Caelo	Sodium perborate, hyd...	13050807	1
Caelo	Sodium perborate, hyd...	13050801	2
Caelo	Sodium perborate, hyd...	13050805	1
Caelo	Sodium sulfate decahy...	12157012	18
Caelo	Sodium sulfate decahy...	205026	1
Caelo	Sodium sulfate decahy...	61599506	1
Caelo	Sodium sulfate decahy...	12157013	1
Caelo	Sodium sulfate decahy...	12157001	1
Caelo	Sodium sulfate decahy...	12157007	1
Caelo	Sodium sulfate decahy...	11012210	2
Caelo	Sodium sulfate decahy...	70706387	1
Caelo	Sodium sulfate decahy...	18101202	1
Caelo	Sodium sulfate decahy...	12157005	13
Caelo	Sodium sulfate decahy...	12157006	3
Caelo	Sodium sulfate decahy...	12256902	1
Caelo	Sodium sulfate decahy...	12257901	1
Caelo	Sodium sulfate decahy...	12157011	1
Caelo	Sodium sulfate decahy...	11012207	1
Caelo	Sodium thiosulfate pe...	26041302	1
Caelo	Sodium thiosulfate pe...	80426288	1
Caelo	Solanum dulcamara ste...	103745604	1
Caelo	Solanum dulcamara ste...	10375605	1
Caelo	Solanum dulcamara ste...	132564301	1
Caelo	Solanum dulcamara ste...	13254301	1
Caelo	Sorrel herb, cut	130546	1
Caelo	Sorrel herb, cut	13289502	2
Caelo	Sour cherry stems, cut	12042301	1
Caelo	Sour cherry stems, cut	10367019	1
Caelo	Sour cherry stems, cut	12042307	1
Caelo	Sour cherry stems, cut	10367014	1
Caelo	Spearmint leaf, cut	13105001	10
Caelo	Spearmint leaf, cut	12133909	1
Caelo	Spearmint leaf, cut	12133901	3
Caelo	Spearmint leaf, cut	1512Q-01505	1
Caelo	Spearmint leaf, cut	11037409+110374	1
Caelo	Spearmint leaf, cut	12376706	1
Caelo	Spearmint leaf, cut	13105003	1
Caelo	Spearmint leaf, cut	12133906	2

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Supplier	Substance	Batch	Spectra
Caelo	St. John's wort, cut	15068105	1
Caelo	St. John's wort, cut	12092209	2
Caelo	St. John's wort, cut	1185608	1
Caelo	St. John's wort, cut	16041301	1
Caelo	St. John's wort, cut	11185602	1
Caelo	St. John's wort, cut	111185608	1
Caelo	St. John's wort, cut	11185607	1
Caelo	St. John's wort, cut	12092201	1
Caelo	St. John's wort, cut	12092204	1
Caelo	St. John's wort, cut	13203204	6
Caelo	St. John's wort, cut	13203205	1
Caelo	St. John's wort, cut	4021B110321	1
Caelo	St. John's wort, cut	268913	1
Caelo	St. John's wort, cut	5021301	1
Caelo	St. John's wort, cut	30011401	1
Caelo	St. John's wort, cut	132203204	1
Caelo	St. John's wort, cut	11185608	18
Caelo	St. John's wort, cut	13091303	1
Caelo	Star anise	11314103	1
Caelo	Star anise	11314104	1
Caelo	Star anise	10376403	2
Caelo	Star anise	10169101	1
Caelo	Star anise	10376405	1
Caelo	Star anise	12226211	1
Caelo	Star anise, cut	16253201	2
Caelo	Stemless carline root	12232803	1
Caelo	Stemless carline root	13130301	6
Caelo	Stemless carline root	23071203	1
Caelo	Stemless carline root	14347401	1
Caelo	Stemless carline root	13130304	1
Caelo	Stemless carline root	25111306	1
Caelo	Stemless carline root	13033501	1
Caelo	Stemless carline root	13130303	1
Caelo	Stemless carline root	12144804	1
Caelo	Strawberry leaf, cut	5122013c	1
Caelo	Strawberry leaf, cut	11117909	1
Caelo	Sulfamerazine	10218401	1
Caelo	Sweet woodruff herb, ...	52236077	1
Caelo	Sweet woodruff herb, ...	10375812	1
Caelo	Sweet woodruff herb, ...	10375802	1
Caelo	Sweet woodruff herb, ...	12103514	1
Caelo	Sweet woodruff herb, ...	18031304	1
Caelo	Sweet woodruff herb, ...	12103509	1
Caelo	Sweet woodruff herb, ...	12103510	1
Caelo	Sweet woodruff herb, ...	12103513	2
Caelo	Sweet woodruff herb, ...	4409M-01621	1
Caelo	Talcum	13146307	1
Caelo	Talcum	12267401	1
Caelo	Talcum	13146308	1
Caelo	Tall golden rod, cut	17091203	1
Caelo	Tall golden rod, cut	11280301	4
Caelo	Tall golden rod, cut	20111209	1
Caelo	Tall golden rod, cut	112080308	1
Caelo	Tall golden rod, cut	265283	1
Caelo	Tall golden rod, cut	15061203	1
Caelo	Tall golden rod, cut	11207010	3
Caelo	Tall golden rod, cut	11280310	6
Caelo	Tall golden rod, cut	12319003	19
Caelo	Tall golden rod, cut	11280308	9
Caelo	Tall golden rod, cut	11280309	1

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Supplier	Substance	Batch	Spectra
Caelo	Tall golden rod, cut	4113A-01684	1
Caelo	Tall golden rod, cut	12319002	2
Caelo	Tall golden rod, cut	13386903	1
Caelo	Tall golden rod, cut	12343109	1
Caelo	Tall golden rod, cut	4021405	1
Caelo	Tall golden rod, cut	27121302	1
Caelo	Tall golden rod, cut	12343105	1
Caelo	Tall golden rod, cut	12343106	1
Caelo	Tall golden rod, cut	14112012	1
Caelo	Tall golden rod, cut	12343103	17
Caelo	Tall golden rod, cut	2656153	1
Caelo	Tall golden rod, cut	13386901	1
Caelo	Tall golden rod, cut	12319006	3
Caelo	Tall golden rod, cut	4091302	1
Caelo	Tall golden rod, cut	12343104	5
Caelo	Tall golden rod, cut	12336801	1
Caelo	Tall golden rod, cut	6081302	1
Caelo	Tall golden rod, cut	12343101	3
Caelo	Tall golden rod, cut	28051302	1
Caelo	Tall golden rod, cut	12319004	10
Caelo	Tall golden rod, cut	12319007	19
Caelo	Tall golden rod, cut	314050-1-p	1
Caelo	Tall golden rod, cut	12343102	3
Caelo	Tall golden rod, cut	14018404	1
Caelo	Tall hawkweed, cut	3611b111005	1
Caelo	Tall nasturtium herb,...	12031605	1
Caelo	Tall nasturtium herb,...	13104406	1
Caelo	Tall nasturtium herb,...	13104405	1
Caelo	Tall nasturtium herb,...	13104404	2
Caelo	Tall nasturtium herb,...	12031603	1
Caelo	Tall nasturtium herb,...	13104403	5
Caelo	Tall nasturtium herb,...	12031601	1
Caelo	Tall nasturtium herb,...	13104402	2
Caelo	Tall nasturtium herb,...	12031602	1
Caelo	Tall nasturtium herb,...	107063	1
Caelo	Tall nasturtium herb,...	13104401	4
Caelo	Tall nasturtium herb,...	12031604	2
Caelo	Tall nasturtium herb,...	12031606	1
Caelo	Theriac, powdered	12189404	2
Caelo	Theriac, powdered	12189401	1
Caelo	Theriac, powdered	11082413	1
Caelo	Theriac, powdered	2021301	1
Caelo	Theriac, powdered	15312504	1
Caelo	Theriac, powdered	12289301	4
Caelo	Theriac, powdered	12289303	1
Caelo	Theriac, powdered	12289306	1
Caelo	Theriac, powdered	12289305	2
Caelo	Theriac, powdered	12289307	8
Caelo	Theriac, powdered	15101307	1
Caelo	Theriac, powdered	412091-2P	1
Caelo	Theriac, powdered	12289312	1
Caelo	Theriac, powdered	13407304	2
Caelo	Theriac, powdered	14156501	1
Caelo	Theriac, powdered	15026401	1
Caelo	Theriac, powdered	11081515	1
Caelo	Theriac, powdered	15312501	1
Caelo	Theriac, powdered	1531501	1
Caelo	Theriac, powdered	15312508	1
Caelo	Thiomersal	10296413	1
Caelo	Thyme, rubbed	13011402	1

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Supplier	Substance	Batch	Spectra
Caelo	Thyme, rubbed	26021301	1
Caelo	Thyme, rubbed	11345004	4
Caelo	Thyme, rubbed	11121306	1
Caelo	Thyme, rubbed	8061206	1
Caelo	Thyme, rubbed	11345002	1
Caelo	Thyme, rubbed	13048309-3475312161	1
Caelo	Thyme, rubbed	10365815	2
Caelo	Thyme, rubbed	13048309	4
Caelo	Thyme, rubbed	15101201	1
Caelo	Thyme, rubbed	13048308	2
Caelo	Thyme, rubbed	4021512	1
Caelo	Thyme, rubbed	13048314	1
Caelo	Thyme, rubbed	14119001	1
Caelo	Thyme, rubbed	15104401	1
Caelo	Thyme, rubbed	10365816	1
Caelo	Thyme, rubbed	10365807	2
Caelo	Thyme, rubbed	23021304	1
Caelo	Thyme, rubbed	16011401	1
Caelo	Thyme, rubbed	13048302	2
Caelo	Thyme, rubbed	29101301	1
Caelo	Thyme, rubbed	13048301	14
Caelo	Thyme, rubbed	22021301	1
Caelo	Thyme, rubbed	11021301	1
Caelo	Thyme, rubbed	29011303	1
Caelo	Thyme, rubbed	11345010	6
Caelo	Thyme, rubbed	11345001	1
Caelo	Thyme, rubbed	21121204	1
Caelo	Thyme, rubbed	11345011	12
Caelo	Thyme, rubbed	4041301	1
Caelo	Thyme, rubbed	25091304	1
Caelo	Thyme, rubbed	11345006	3
Caelo	Thyme, rubbed	11345007	5
Caelo	Thyme, rubbed	11345014	12
Caelo	Thyme, rubbed	25041302	1
Caelo	Thyme, rubbed		1
Caelo	Thyme, rubbed	11345013	6
Caelo	Thyme, rubbed	12111201	1
Caelo	Thyme, rubbed	1134514	1
Caelo	Thyme, rubbed	13081301	1
Caelo	Tonka beans	12144101	1
Caelo	Tonka beans	1078C	1
Caelo	Tonka beans	12145101	2
Caelo	Tonka beans	20111312	1
Caelo	Tormentil	30011405	1
Caelo	Tormentil	25022014A	1
Caelo	Tormentil	12040713	1
Caelo	Tormentil	12216801	4
Caelo	Tormentil	14008002	2
Caelo	Tormentil	14008001	2
Caelo	Tormentil	12040717	1
Caelo	Tormentil	14140001	1
Caelo	Tormentil	14008005	1
Caelo	Tormentil	2512A-02188	1
Caelo	Tormentil	1914A-02188	1
Caelo	Tormentil	12040708	9
Caelo	Tormentil	10081203	1
Caelo	Tormentil	12040704	2
Caelo	Tormentil	11102010	1
Caelo	Tormentil	15085501	1
Caelo	Tormentil	14360103	1

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Supplier	Substance	Batch	Spectra
Caelo	Tormentil	15178202	2
Caelo	Tormentil	15178203	1
Caelo	Tormentil	15178206	1
Caelo	Tormentil	12216802	1
Caelo	Tormentil	12040707	1
Caelo	Tormentil	15364302	4
Caelo	Tormentil	12216805	1
Caelo	Tormentil	411082-2-P	1
Caelo	Tormentil	13220502	1
Caelo	Tormentil	4753268	1
Caelo	Tormentil	12216803	4
Caelo	Tragacanth, powdered	1327802	1
Caelo	Tragacanth, powdered	13095203	1
Caelo	Tragacanth, powdered	15041302	1
Caelo	Tragacanth, powdered	1228503	1
Caelo	Tragacanth, powdered	12285403	3
Caelo	Tragacanth, powdered	11128905	1
Caelo	Tragacanth, powdered	12285402	1
Caelo	Tragacanth, powdered	13095208	3
Caelo	Tragacanth, powdered	15121203	1
Caelo	Tragacanth, powdered	8081201	1
Caelo	Tragacanth, powdered	14011302	1
Caelo	Tragacanth, powdered	13277802	4
Caelo	Tragacanth, powdered	16350004	1
Caelo	Tragacanth, powdered	16110802	1
Caelo	Tragacanth, powdered	13277804	3
Caelo	Tragacanth, powdered	14162205	7
Caelo	Tragacanth, powdered	15085602	4
Caelo	Tragacanth, powdered	15085602	1
Caelo	Tragacanth, powdered	15085606	6
Caelo	Tragacanth, powdered	9081202	1
Caelo	Tragacanth, powdered	16110807	1
Caelo	Tragacanth, powdered	14162207	1
Caelo	Tragacanth, powdered	15085607	1
Caelo	Tragacanth, powdered	13204705	6
Caelo	Tragacanth, powdered	153799	1
Caelo	Tragacanth, powdered	20111305	1
Caelo	Tragacanth, powdered	13204701	4
Caelo	Tragacanth, powdered	12285408	1
Caelo	Tragacanth, powdered	7021402	1
Caelo	Tragacanth, powdered	12108806	1
Caelo	Trichloroacetic acid	13056213	1
Caelo	Trichloroacetic acid	10379401	1
Caelo	Trichloroacetic acid	14101711	1
Caelo	Trichloroacetic acid	12135210	1
Caelo	Trichloroacetic acid	13056212	1
Caelo	Trichloroacetic acid	6091306	1
Caelo	Trichloroacetic acid	13056209	1
Caelo	Trichloroacetic acid	13056203	3
Caelo	Trichloroacetic acid	12135203	1
Caelo	Trichloroacetic acid	11294318	1
Caelo	Trichloroacetic acid	12g04m11	1
Caelo	Trichloroacetic acid	12135201	1
Caelo	Trichloroacetic acid	12135207	5
Caelo	Trichloroacetic acid	10130802	1
Caelo	Turmeric root, cut	15372603	1
Caelo	Turmeric root, cut	15158001	2
Caelo	Turmeric root, cut	12136501	2
Caelo	Turmeric root, cut	15207601	1
Caelo	Turmeric root, cut	15158001	2

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Supplier	Substance	Batch	Spectra
Caelo	Turmeric root, cut	13360204	2
Caelo	Turmeric root, cut	12136503	2
Caelo	Turmeric root, cut	1213650	1
Caelo	Turmeric root, cut	12136506	1
Caelo	Turmeric root, cut	12136504	1
Caelo	Turmeric root, cut	12136507	1
Caelo	Turmeric, javanese, cut	11182903	1
Caelo	Turmeric, javanese, cut	13262907	1
Caelo	Turmeric, javanese, cut	15120202	2
Caelo	Turmeric, javanese, cut	25041313	1
Caelo	Turmeric, javanese, cut	14309503	1
Caelo	Turmeric, javanese, cut	17042003	1
Caelo	Turmeric, javanese, cut	12319206	2
Caelo	Turmeric, javanese, cut	12319206	2
Caelo	Turmeric, javanese, cut	14017706	1
Caelo	Turmeric, javanese, cut	12319201	1
Caelo	Valerian root, cut	11349101	4
Caelo	Valerian root, cut	11103602	1
Caelo	Valerian root, cut	11103601	1
Caelo	Valerian root, cut	11103608	1
Caelo	Valerian root, cut	11103609	4
Caelo	Valerian root, cut	13119003	12
Caelo	Valerian root, cut	28101303	1
Caelo	Valerian root, cut	120338012	1
Caelo	Valerian root, cut	1319003	1
Caelo	Valerian root, cut	13119004	3
Caelo	Valerian root, cut	20081303	1
Caelo	Valerian root, cut	29101303	1
Caelo	Valerian root, cut	13196802	4
Caelo	Valerian root, cut	13196806	6
Caelo	Valerian root, cut	13196801-3564412081	1
Caelo	Valerian root, cut	13287402	3
Caelo	Valerian root, cut	15175205	1
Caelo	Valerian root, cut	13119002	18
Caelo	Valerian root, cut	13119001	1
Caelo	Valerian root, cut	12033811	5
Caelo	Valerian root, cut	12033807	1
Caelo	Valerian root, cut	12033809	9
Caelo	Valerian root, cut	12033808	5
Caelo	Valerian root, cut	2712A-02167	1
Caelo	Valerian root, cut	12033805	4
Caelo	Valerian root, cut	31121201	1
Caelo	Valerian root, cut	11103607	3
Caelo	Valerian root, cut	31101202	1
Caelo	Valerian root, cut	11035002	1
Caelo	Valerian root, cut	3091202	1
Caelo	Valerian root, cut	11103612	2
Caelo	Valerian root, cut	12033812	8
Caelo	Valerian root, cut	12033810	1
Caelo	Valerian root, powdered	13287402	2
Caelo	Valerian root, powdered	15175204	1
Caelo	Verbena herb, cut	4651b120611	1
Caelo	Verbena herb, cut	11031105	2
Caelo	Verbena herb, cut	13151001	15
Caelo	Verbena herb, cut	12383002	2
Caelo	Verbena herb, cut	12178601	1
Caelo	Verbena herb, cut	13151003	5
Caelo	Verbena herb, cut	12383005	1
Caelo	Verbena herb, cut	2x12188202	1
Caelo	Verbena herb, cut	13351401	1

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Supplier	Substance	Batch	Spectra
Caelo	Verbena herb, cut	15012405	1
Caelo	Verbena herb, cut	12188202	10
Caelo	Verbena herb, cut	12187601	14
Caelo	Verbena herb, cut	110031110	1
Caelo	Verbena herb, cut	19111205	1
Caelo	Verbena herb, cut	11031103	1
Caelo	Verbena herb, cut	11031108	5
Caelo	Verbena herb, cut	11031106	5
Caelo	Verbena herb, cut	12188203	5
Caelo	Verbena herb, cut	6111301	1
Caelo	Verbena herb, cut	11031110	6
Caelo	Walnut bark, cut	11325606	1
Caelo	Walnut bark, cut	11016604	1
Caelo	Walnut bark, cut	11016605	1
Caelo	Walnut bark, cut	11325603	1
Caelo	Walnut leaf, cut	12124601	5
Caelo	Walnut leaf, cut	1414Q01499	1
Caelo	Walnut leaf, cut	12124605	6
Caelo	Walnut leaf, cut	414Q1499	1
Caelo	Walnut leaf, cut	12124602	3
Caelo	Walnut leaf, cut	4713U01499	1
Caelo	Walnut leaf, cut	12124603-341930192	1
Caelo	Walnut leaf, cut	3712Q-01499	1
Caelo	Walnut leaf, cut	3051301	1
Caelo	Walnut leaf, cut	11103010	5
Caelo	Walnut leaf, cut	11103008	4
Caelo	Walnut leaf, cut	11103007	5
Caelo	Walnut leaf, cut	10050416	1
Caelo	Walnut leaf, cut	1214603	1
Caelo	Walnut leaf, cut	11103004	2
Caelo	Walnut leaf, cut	11103003	2
Caelo	Walnut leaf, cut	14064904	1
Caelo	Walnut leaf, cut	15126008	5
Caelo	Walnut leaf, cut	12124502	1
Caelo	Walnut leaf, cut	15126003	6
Caelo	Walnut leaf, cut	14064902	4
Caelo	Walnut leaf, cut	14064906	3
Caelo	Walnut leaf, cut	14064909	1
Caelo	Walnut leaf, cut	15126004	1
Caelo	Walnut leaf, cut	14064903	1
Caelo	Walnut leaf, cut	14064910	1
Caelo	White deadnettle flower	10081206	1
Caelo	White deadnettle flower	12152402	2
Caelo	White deadnettle flower	11371610	5
Caelo	White deadnettle flower	11371609	3
Caelo	White deadnettle flower	52470437	1
Caelo	White deadnettle flower	2101301	1
Caelo	White deadnettle flower	11371613	2
Caelo	White deadnettle flower	12275802	1
Caelo	White deadnettle flower	15299101	1
Caelo	White deadnettle flower	11371611	2
Caelo	White deadnettle herb...	11371703	1
Caelo	White deadnettle herb...	11371706	3
Caelo	White deadnettle herb...	11371711	2
Caelo	White deadnettle herb...	11371712	1
Caelo	White deadnettle herb...	11371705	1
Caelo	White deadnettle herb...	11371709	1
Caelo	White deadnettle herb...	11371702	1
Caelo	White mustard seed, p...	13224804	3
Caelo	White mustard seed, p...	7254a110823	1

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Supplier	Substance	Batch	Spectra
Caelo	White mustard seed, p...	13224801	1
Caelo	White mustard seed, p...	12375704	1
Caelo	White mustard seed, p...	12375706	2
Caelo	White mustard seed, p...	12375705	1
Caelo	White mustard seed, p...	12375702	1
Caelo	White mustard seed, p...	12375701	1
Caelo	White mustard seed, p...	11114409	1
Caelo	White mustard seed, p...	12375705	4
Caelo	Wild apple, sweet	11229805	1
Caelo	Wild pansy, cut	12382806	1
Caelo	Wild pansy, cut	12382802	1
Caelo	Wild pansy, cut	12189204-3463312101	1
Caelo	Wild pansy, cut	12189204-3458312120	1
Caelo	Wild pansy, cut	7101303	1
Caelo	Wild pansy, cut	12189204	10
Caelo	Wild pansy, cut	10291007	1
Caelo	Wild pansy, cut	17101205	1
Caelo	Wild pansy, cut	5021304	1
Caelo	Wild pansy, cut	15021301	1
Caelo	Wild pansy, cut	12189203	5
Caelo	Wild pansy, cut	11216103	2
Caelo	Wild pansy, cut	13091205	1
Caelo	Wild pansy, cut	12189203	4
Caelo	Wild pansy, cut	14061311	1
Caelo	Wild pansy, cut	10291009	3
Caelo	Wild pansy, cut	1289203	1
Caelo	Wild pansy, cut	12189204	4
Caelo	Wild thyme, cut	13086805	3
Caelo	Wild thyme, cut	4501A120813	2
Caelo	Wild thyme, cut	11374803	1
Caelo	Wild thyme, cut	11374805i.0.	1
Caelo	Wild thyme, cut	11374805	4
Caelo	Wild thyme, cut	11031203	1
Caelo	Willow bark, cut	12185207	3
Caelo	Willow bark, cut	13180705	1
Caelo	Willow bark, cut	11073208	1
Caelo	Willow bark, cut	2185206	1
Caelo	Willow bark, cut	12185208	12
Caelo	Willow bark, cut	13180701	1
Caelo	Willow bark, cut	9071301	1
Caelo	Willow bark, cut	13180702	4
Caelo	Willow bark, cut	13180705-3530411072	1
Caelo	Willow bark, cut	12185201	5
Caelo	Willow bark, cut	11073201	1
Caelo	Willow bark, cut	21011302	1
Caelo	Willow bark, cut	12185204	4
Caelo	Willow bark, cut	12185206	5
Caelo	Willow bark, cut	11073210	3
Caelo	Willow herb, cut	13104702	1
Caelo	Willow herb, cut	13200203	1
Caelo	Willow herb, cut	11347311	1
Caelo	Willow herb, cut	11347318	2
Caelo	Willow herb, cut	11347316	1
Caelo	Willowherb, small flo...	29121201	1
Caelo	Willowherb, small flo...	12064506	1
Caelo	Willowherb, small flo...	18031305	1
Caelo	Willowherb, small flo...	1031301	1
Caelo	Willowherb, small flo...	28031318	1
Caelo	Willowherb, small flo...	13200202-3481312102	1
Caelo	Willowherb, small flo...	13200201	3

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Supplier	Substance	Batch	Spectra
Caelo	Willowherb, small flo...	13200203	7
Caelo	Willowherb, small flo...	2081305	1
Caelo	Willowherb, small flo...	12117701	8
Caelo	Willowherb, small flo...	12117701-3371319012	1
Caelo	Willowherb, small flo...	12041301	1
Caelo	Willowherb, small flo...	10326104	4
Caelo	Willowherb, small flo...	21061307	1
Caelo	Willowherb, small flo...	13071301	1
Caelo	Willowherb, small flo...	16081304	1
Caelo	Willowherb, small flo...	16081302	1
Caelo	Willowherb, small flo...	412041	1
Caelo	Willowherb, small flo...	7071201	1
Caelo	Willowherb, small flo...	9378908	1
Caelo	Willowherb, small flo...	2412E-01641	1
Caelo	Willowherb, small flo...	10326108	14
Caelo	Willowherb, small flo...	15101302	1
Caelo	Willowherb, small flo...	15011411	1
Caelo	Willowherb, small flo...	31101303	1
Caelo	Willowherb, small flo...	14267909	1
Caelo	Willowherb, small flo...	13355906	2
Caelo	Wormwood herb, cut	15408304	1
Caelo	Wormwood herb, cut	13381905	1
Caelo	Wormwood herb, cut	13381902	3
Caelo	Wormwood herb, cut	7011401	1
Caelo	Wormwood herb, cut	13174402	1
Caelo	Wormwood herb, cut	13174401	3
Caelo	Wormwood herb, cut	12355807	10
Caelo	Wormwood herb, cut	277513	1
Caelo	Wormwood herb, cut	12355804	8
Caelo	Wormwood herb, cut	12355805	4
Caelo	Wormwood herb, cut	12355802	3
Caelo	Wormwood herb, cut	7031301	1
Caelo	Wormwood herb, cut	12355808	2
Caelo	Wormwood herb, cut	12355803	26
Caelo	Wormwood herb, cut	12355801	20
Caelo	Wormwood herb, cut	272957	1
Caelo	Wormwood herb, cut	6101203	1
Caelo	Wormwood herb, cut	11285810	6
Caelo	Wormwood herb, cut	11285805	2
Caelo	Wormwood herb, cut	11285802	2
Caelo	Wormwood herb, cut	11285803	1
Caelo	Yarrow flower, rubbed	13350507	1
Caelo	Yarrow flower, rubbed	12363005	5
Caelo	Yarrow flower, rubbed	70139427	1
Caelo	Yarrow flower, rubbed	12338306	1
Caelo	Yarrow flower, rubbed	12267702	1
Caelo	Yarrow flower, rubbed	12363002	6
Caelo	Yarrow flower, rubbed	12267703	2
Caelo	Yarrow herb, cut	12338305	7
Caelo	Yarrow herb, cut	12338304	15
Caelo	Yarrow herb, cut	12338303	8
Caelo	Yarrow herb, cut	5021302	1
Caelo	Yarrow herb, cut	11306301	1
Caelo	Yarrow herb, cut	10101205	1
Caelo	Yarrow herb, cut	11218404	1
Caelo	Yarrow herb, cut	11280514	2
Caelo	Yarrow herb, cut	11280517	1
Caelo	Yarrow herb, cut	11280511	2
Caelo	Yarrow herb, cut	11280512	9
Caelo	Yarrow herb, cut	12336306	1

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Supplier	Substance	Batch	Spectra
Caelo	Yarrow herb, cut	12379602	9
Caelo	Yarrow herb, cut	27011404	1
Caelo	Yarrow herb, cut	12338311	2
Caelo	Yarrow herb, cut	13029105	4
Caelo	Yarrow herb, cut	12338306-3358319071	1
Caelo	Yarrow herb, cut	9101311	1
Caelo	Yarrow herb, cut	16102013E	1
Caelo	Yarrow herb, cut	1309106	1
Caelo	Yarrow herb, cut	12379603	7
Caelo	Yarrow herb, cut	15006708	1
Caelo	Yarrow herb, cut	15006720	1
Caelo	Yarrow herb, cut	15006713	1
Caelo	Yarrow herb, cut	13029107-3436311151	1
Caelo	Yarrow herb, cut	1408510	1
Caelo	Yarrow herb, cut	14018503	2
Caelo	Yarrow herb, cut	13381805	1
Caelo	Yarrow herb, cut	13381810	1
Caelo	Yarrow herb, cut	12379606	9
Caelo	Yarrow herb, cut	9121304	1
Caelo	Yarrow herb, cut	130929105	1
Caelo	Yarrow herb, cut	13381806	2
Caelo	Yarrow herb, cut	12379607	1
Caelo	Yarrow herb, cut	8011421	1
Caelo	Yarrow herb, cut	13029106	10
Caelo	Yarrow herb, cut	13029107-3418310182	1
Caelo	Yarrow herb, cut	10081301	1
Caelo	Yarrow herb, cut	13029108	9
Caelo	Yarrow herb, cut	12041302	1
Caelo	Yarrow herb, cut	16041302	1
Caelo	Yarrow herb, cut	12379601	8
Caelo	Yarrow herb, cut	13029103	12
Caelo	Yarrow herb, cut	13029104	5
Caelo	Yarrow herb, cut	29071301	1
Caelo	Yarrow herb, cut	H-220313-1	1
Caelo	Yellow chaste weed, cut	11293101	4
Caelo	Yellow chaste weed, cut	10244407	1
Caelo	Yellow chaste weed, cut	12170602	2
Caelo	Yellow chaste weed, cut	12170603	1
Caelo	Yellow chaste weed, cut	15029505	1
Caelo	Yellow chaste weed, cut	12170605	2
Caelo	Yellow chaste weed, cut	1024407	1
Caelo	Yellow chaste weed, cut	512U-01473	1
Caelo	Zedoary root, cut	11091603	1
Caelo	Zedoary root, cut	111091607	1
Caelo	Zedoary root, cut	12125301	3
Caelo	Zedoary root, cut	12125304	2
Caelo	Zedoary root, cut	13010102	3
Caelo	Zedoary root, cut	13010104	1
Caelo	Zedoary root, cut	25111304	1
Caelo	Zedoary root, powdered	12007504	1
Caelo	Zedoary root, powdered	13165501	2
Caelo	Zedoary root, powdered	13165504	4
Caelo	Zedoary root, powdered	15277101	1
Caelo	Zedoary root, powdered	15352606	1
Caelo	Zinc sulfate heptahyd...	12257809	2
Caelo	Zinc sulfate heptahyd...	4012Q-02798	1
Caelo	Zinc sulfate heptahyd...	12257816	1
Caelo	Zinc sulfate heptahyd...	11095621	1
Caelo	Zinc sulfate heptahyd...	81554199	1
Caelo	Zinc sulfate heptahyd...	12257802	1

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Supplier	Substance	Batch	Spectra
Caelo	Zinc sulfate heptahyd...	11095601	1
Caelo	Zinc sulfate heptahyd...	12257818	1
Caesar & Lorenz	Yarrow herb, cut	12379605	3
Caesar & Loretz GmbH	Hawthorn flower	11068206	3
Caesar & Loretz GmbH	Magnesium chloride he...	13064223	1
Caesar & Loretz GmbH	Morphine hydrochloride	15199711(2)	1
Caesar & Loretz GmbH	Morphine hydrochloride	15199712	1
Caesar & Loretz GmbH	Morphine hydrochloride	15199711	1
Caesar & Loretz GmbH	Morphine hydrochloride	15199711(1)	1
Caesar & Loretz GmbH	Peppermint leaf, cut	11294411	1
Caesar & Loretz GmbH	Thiomersal	12275218	1
Caesar & Loretz GmbH ...	Bitter fennel	11016331	1
Caesar & Loretz GmbH ...	Potassium hydroxide	12057902	2
Caesar & Loretz GmbH ...	Sage leaf, cut	11056121	3
Caesar & Loretz GmbH,...	Aluminium chloride he...	12323702	14
Caesar & Loretz GmbH,...	Aluminium chloride he...	12047508	4
Caesar & Loretz GmbH,...	Birch leaf, cut	11050102	3
Caesar & Loretz GmbH,...	Bitter fennel	11016319	1
Caesar & Loretz GmbH,...	Caraway fruit	11003213	2
Caesar & Loretz GmbH,...	Caraway fruit	9267824	2
Caesar & Loretz GmbH,...	Equisetum stem, cut	12288801	14
Caesar & Loretz GmbH,...	Equisetum stem, cut	10375510	2
Caesar & Loretz GmbH,...	Gentian root, cut	12244603	2
Caesar & Loretz GmbH,...	Liquorice root, peeled	11034014	1
Caesar & Loretz GmbH,...	Lungwort herb, cut	13029304	5
Caesar & Loretz GmbH,...	Mallow flower, cut	12187402	7
Caesar & Loretz GmbH,...	Mallow flower, cut	13267301	5
Caesar & Loretz GmbH,...	Maté leaf, cut	13118002	10
Caesar & Loretz GmbH,...	Nettle leaf, cut	10291423	6
Caesar & Loretz GmbH,...	Raspberry leaf, cut	10013408	1
Caesar & Loretz GmbH,...	Ribwort plantain, cut	12362903	29
Caesar & Loretz GmbH,...	Ribwort plantain, cut	13113004	10
Caesar & Loretz GmbH,...	Sage leaf, cut	11347502	5
Caesar & Loretz GmbH,...	Sage leaf, cut	12370002	4
Caesar & Loretz GmbH,...	Sage leaf, cut	12370010	16
Caesar & Loretz GmbH,...	Sage leaf, cut	12370016	8
Caesar & Loretz GmbH,...	Senna leaf, cut	11277308	3
Caesar & Loretz GmbH,...	Senna leaf, cut	11277303	3
Caesar & Loretz GmbH,...	Senna leaf, cut	13136708	7
Caesar & Loretz GmbH,...	Senna leaf, cut	11277314	5
Caesar & Loretz GmbH,...	Senna leaf, cut	12273103	11
Caesar & Loretz GmbH,...	Senna pods, tinnevelly	12267601	2
Caesar & Loretz GmbH,...	Senna pods, tinnevelly	11003014	1
Caesar & Loretz GmbH,...	Senna pods, tinnevelly	11003012	1
Caesar & Loretz GmbH,...	Senna pods, tinnevelly	12267603	1
Caesar & Loretz GmbH,...	Sodium hydrogen carbo...	13060102	1
Caesar & Loretz GmbH,...	Tall golden rod, cut	11207014	3
Caesar & Loretz GmbH,...	Wild thyme, cut	11374802	1
Caesar & Loretz GmbH,...	Yarrow herb, cut	12338306	3
Caesar & Loretz/ Noweda	Heavy alkaline bismut...	12145701	1
Caesar & Loretz/ Noweda	Hyssop herb, cut	11374301	1
Caesar & Loretz/ Noweda	Ivy leaf, cut	12225606	5
Caesar & Loretz/Noweda	Aniseed	153986002	1
Caesar & Loretz/Noweda	Caraway fruit	15056601	1
Caesar&Loretz GmbH D-...	Senna leaf, cut	12115504	4
Caesar&Loretz,Anzag	Sodium monohydrogenph...	12256606	3
Caesar&Loretz,Phoenix	Frangula bark, cut	14163104	1
Caesar&Loretz,Phoenix	Ladys bedstraw herb,...	14019215	1
Caesar&Loretz,Phoenix	Ladys bedstraw herb,...	14019206	1
Caesar&Loretz,Phoenix	Marjoram herb, rubbed	14181005	1

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Supplier	Substance	Batch	Spectra
caesar&lorenz,Phönix	Iceland moss, cut	14304404	3
Caesar/ Noweda	Black mustard seed, p...	14293711	3
Caesar/Noweda	Aloes, cape, cut	2013E-01089	1
Caesar/Noweda	Aloes, cape, cut	12338211	1
Caesar/Noweda	Aluminium potassium s...	12184411	2
Caesar/Noweda	American liverwort, cut	11254608	1
Caesar/Noweda	Bogbean leaf, cut	1510U-01517	1
Caesar/Noweda	Coriander	2010M-01539	1
Caesar/Noweda	Couch grass rhizome, ...	12186813	4
Caesar/Noweda	Elder flower, rubbed	4910A-01471	1
Caesar/Noweda	Heather, cut	4911I-03224	1
Caesar/Noweda	Ispaghula seed	12276503	1
Caesar/Noweda	Ispaghula seed	12276509	3
Caesar/Noweda	Ispaghula seed	12276516	1
Caesar/Noweda	Lycopodium herb, cut	1255008	1
Caesar/Noweda	Mullein flower, cut	2810E-01475	1
Caesar/Noweda	Psyllium seed	11185817	3
Caesar/Noweda	Psyllium seed	12276501	3
Caesar/Noweda	Restharrow root, cut	71015/3	2
Caesar/Noweda	Theriac, powdered	12289309	1
Cealo	Ispaghula seed	12276502	4
Cealo	Magnesium chloride he...	112354615	1
Cealo	Magnesium chloride he...	11354615	1
Cealo	Ribwort plantain, cut	12362907	1
Cealo	Senna leaf, cut	12273116	15
Cealo/ Noweda	Midazolam hydrochloride	17168006	2
Cealo/Gehe	Tormentil	14140006	3
Celo	Agrimony, cut	11374003	1
Chiesi/Phönix	Black cumin seed	14359906	2
China Medica	Raspberry leaf, cut	13086703	1
Clariant - Mindel-Food	Bentonite	1301	1
Creapure	Creatine	515941	1
Defektur	Bitter fennel	7/13	1
Defektur	Bitter fennel	57/13	1
Defektur	Bitter fennel	52/13	1
Defektur	Matricaria flower	59/13	1
Defektur	Matricaria flower	29/13	1
Defektur	Matricaria flower	56/12	1
Defektur	Matricaria flower	10/13	1
Degussa / falceto	Creatine	422031	1
Dermapharm	8-quinolinol sulfate ...	140804	1
Dermapharm	8-quinolinol sulfate ...	100804	1
Dermapharm	8-quinolinol sulfate ...	120905	1
Dr. Behr	Dimercaptosuccinic acid	WE14020002	1
Dr. Wolff	Methadone hydrochloride	16F24-B02	1
ebert u.jacobi	Marian thistle fruit	287527	1
Ebert-Jacobi	Methadone hydrochloride	16135306	1
Eu Rho	Sodium hydrogen carbo...	1203030-01	8
EuRho	Aluminium chloride he...	2512I01095	1
EuRho	Aluminium chloride he...	d024a	1
EuRho	Aluminium chloride he...	1106017-01	1
EuRho	Magnesium sulfate hep...	1303008-01	5
EuRho	Magnesium sulfate hep...	3512M-01835	1
EuRho	Sodium sulfate decahy...	1210005-01	2
EuRho Pharm	Aluminium chloride he...	1109025-02	3
Eurho/Phoenix	Midazolam hydrochloride	12L17-N10	1
Euro / Jenne	Magnesium sulfate hep...	1401029-01	2
Euro OCT	Sodium hydrogen carbo...	1307017-01	1
Euro OTC	Almonds, bitter, whole	290973	2
Euro OTC	Aluminium chloride he...	1210014-02-336331909	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Aluminium chloride he...	1213M-01095	1
Euro OTC	Aluminium chloride he...	1507002-01	1
Euro OTC	Aluminium chloride he...	1210014-01	25
Euro OTC	Aluminium chloride he...	2111Q-01095	1
Euro OTC	Aluminium chloride he...	1204026-01	20
Euro OTC	Aluminium chloride he...	120402602	1
Euro OTC	Aluminium chloride he...	1109025-01	1
Euro OTC	Aluminium chloride he...	co31a	1
Euro OTC	Aluminium chloride he...	1210012-01	1
Euro OTC	Aluminium chloride he...	1406021-01	1
Euro OTC	Aluminium chloride he...	1103007-01	1
Euro OTC	Aluminium chloride he...	1307011-02	2
Euro OTC	Aluminium chloride he...	1307011-01	10
Euro OTC	Aluminium chloride he...	1210014-02	28
Euro OTC	Aluminium chloride he...	121001402	1
Euro OTC	Aluminium chloride he...	1307011	1
Euro OTC	Aluminium chloride he...	120402601	3
Euro OTC	Aluminium potassium s...	1004046-02	1
Euro OTC	Ammonium chloride	1212017-01	2
Euro OTC	Ammonium chloride	512A-01104	1
Euro OTC	Ammonium chloride	1303029-01	1
Euro OTC	Ammonium chloride	1203029-01	1
Euro OTC	Angelica root	301767	2
Euro OTC	Betaine hydrochloride	1510011-02	1
Euro OTC	Betaine hydrochloride	L1412019-01	1
Euro OTC	Betaine hydrochloride	L1510011-03	2
Euro OTC	Betaine hydrochloride	1305027-01	2
Euro OTC	Betaine hydrochloride	L1701040-01	1
Euro OTC	Betaine hydrochloride	1202008-01	1
Euro OTC	Chromium yeast 0.2%	L1311026-01	1
Euro OTC	Cysteine hydrochlorid...	1304019-01	1
Euro OTC	Dandelion herb with r...	11030312	4
Euro OTC	Deoxycholic acid	1305051-01	1
Euro OTC	Equisetum stem, cut	3831A130610	5
Euro OTC	Frankincense extract ...	1104005V-04	2
Euro OTC	Hamamelis leaf, cut	12164805	1
Euro OTC	Magnesium carbonate, ...	1305024-01	1
Euro OTC	Magnesium carbonate, ...	1211005-01	4
Euro OTC	Magnesium chloride he...	1204017-01	1
Euro OTC	Magnesium chloride he...	1212013-01	3
Euro OTC	Magnesium chloride he...	1112013-01	2
Euro OTC	Magnesium sulfate hep...	1202017-01	6
Euro OTC	Magnesium sulfate hep...	130300801	1
Euro OTC	Magnesium sulfate hep...	170610	1
Euro OTC	Magnesium sulfate hep...	1109023-01	2
Euro OTC	Magnesium sulfate hep...	1306015-01	1
Euro OTC	Marian thistle herb, ...	3701A-111207	1
Euro OTC	Methadone hydrochloride	14C24-B01	2
Euro OTC	Methadone hydrochloride	16135304	5
Euro OTC	Nettle seed	12131507	2
Euro OTC	Oak bark, cut		1
Euro OTC	Potassium hydrocarbon...	4413I1728	1
Euro OTC	Potassium hydrocarbon...	2809033-01	1
Euro OTC	Potassium hydrocarbon...	1202013-01	1
Euro OTC	Potassium hydrocarbon...	1204038-01	2
Euro OTC	Potassium hydrocarbon...	1208010-01	3
Euro OTC	Sodium alginate	1509036-01	1
Euro OTC	Sodium dihydrogen pho...	1209004-01	2
Euro OTC	Sodium dihydrogen pho...	1305028-01	1
Euro OTC	Sodium hydrogen carbo...	1104013-01	2

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Supplier	Substance	Batch	Spectra
Euro OTC	Sodium hydrogen carbo...	1109029-01	8
Euro OTC	Sodium hydrogen carbo...	120800801	1
Euro OTC	Sodium hydrogen carbo...	1304017-01	5
Euro OTC	Sodium hydrogen carbo...	1012011	1
Euro OTC	Sodium hydrogen carbo...	1304017-02	2
Euro OTC	Sodium hydrogen carbo...	1208008-01	9
Euro OTC	Sodium hydrogen carbo...	120303001	1
Euro OTC	Sodium hydrogen carbo...	1012011-01	1
Euro OTC	Sodium sulfate decahy...	1210005-02	2
Euro OTC	Sodium sulfate decahy...	121000502	2
Euro OTC	Sodium sulfate decahy...	4312I-01920	1
Euro OTC	Sodium sulfate decahy...	1108035-02	2
Euro OTC	Sodium sulfate decahy...	1108035-01	2
Euro OTC	Thyme, rubbed	4622A130109	72
Euro OTC	Tricalcium phosphate	1206002-01	3
Euro OTC	Tricalcium phosphate	1304025-01	1
Euro OTC	Zinc sulfate heptahyd...	1309011_0	1
Euro OTC	Zinc sulfate heptahyd...	1201031-2	1
Euro OTC	Zinc sulfate heptahyd...	1201031-02	1
Euro OTC	Zinc sulfate heptahyd...	1105002-01	1
Euro OTC	Zinc sulfate heptahyd...	1201031-01	1
Euro/ Sanacorp	Codeine phosphate hem...	15F09-B02-315564	2
EUro/AHD	Aluminium chloride he...	121001401	3
EUro/AHD	Calcium chloride dihy...	1205014-02	2
euroho/gehe	Sodium hydrogen carbo...	123030-02	1
Euroo/Phoenix	Aluminium chloride he...	120014-02	1
Faagron	Methadone hydrochloride	1437H011	1
Fagro/ Noweda	Methadone hydrochloride	17/15-B02-339527	1
Fagro//Noweda	Methadone hydrochloride	15/24-B07-317267	1
Fagro/Jenne	Methadone hydrochloride	17I15-B02-339525	2
Fagron	(R,S)-epinephrine hyd...	14A22-B05	1
Fagron	(R,S)-epinephrine hyd...	16H23-B98-325052	1
Fagron	(R,S)-epinephrine hyd...	10022015E	1
Fagron	(R,S)-epinephrine hyd...	2021503	1
Fagron	8-quinolinol sulfate ...	12H21-N08	1
Fagron	8-quinolinol sulfate ...	13G10-N06	1
Fagron	8-quinolinol sulfate ...	11I09-N09	1
Fagron	8-quinolinol sulfate ...	13A04-N05	1
Fagron	8-quinolinol sulfate ...	13D24-N11	1
Fagron	8-quinolinol sulfate ...	10F01-N15	1
Fagron	8-quinolinol sulfate ...	13/21-N23	1
Fagron	8-quinolinol sulfate ...	12D26-N04	1
Fagron	8-quinolinol sulfate ...	11/09-N09	1
Fagron	8-quinolinol sulfate ...	12A04-N05	1
Fagron	8-quinolinol sulfate ...	13032014C	1
Fagron	8-quinolinol sulfate ...	11L19-N14	1
Fagron	8-quinolinol sulfate ...	11L08-N07	2
Fagron	Alchemilla, cut	11182802	1
Fagron	Aluminium chloride he...	5213A1095	1
Fagron	Aluminium chloride he...	11/23-N06B206A	1
Fagron	Aluminium chloride he...	105282-0001	1
Fagron	Aluminium chloride he...	12i27-N01	2
Fagron	Aluminium chloride he...	13J31-B06-287615	1
Fagron	Aluminium chloride he...	C145A	1
Fagron	Aluminium chloride he...	13D22N09	2
Fagron	Aluminium chloride he...	12/27-N01	7
Fagron	Aluminium chloride he...	8547287	1
Fagron	Aluminium chloride he...	11123-N06	3
Fagron	Aluminium chloride he...	13d22no9	1
Fagron	Aluminium chloride he...	C181A	2

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Supplier	Substance	Batch	Spectra
Fagron	Aluminium chloride he...	2013U-01095	1
Fagron	Aluminium chloride he...	12/11-No3	1
Fagron	Aluminium chloride he...	12G05-N10	23
Fagron	Aluminium chloride he...	13126-N13	1
Fagron	Aluminium chloride he...	13D22-N09	26
Fagron	Aluminium chloride he...	12L11-N03	3
Fagron	Aluminium chloride he...	11/23-N06	2
Fagron	Aluminium chloride he...	11 23-N06	1
Fagron	Aluminium chloride he...	12I27-N01	11
Fagron	Aluminium chloride he...	11G05-N02	1
Fagron	Aluminium chloride he...	12I27-N01	4
Fagron	Aluminium chloride he...	12/27/N01	1
Fagron	Aluminium chloride he...	20122013E	1
Fagron	Aluminium chloride he...	C012A	1
Fagron	Aluminium chloride he...	12082013D	1
Fagron	Aluminium chloride he...	11G05-No2	1
Fagron	Aluminium chloride he...	13I26-N13	2
Fagron	Aluminium chloride he...	1910211095	1
Fagron	Aluminium chloride he...	2913U1095	1
Fagron	Aluminium chloride he...	1207211095	1
Fagron	Aluminium chloride he...	12C07-N01	7
Fagron	Aluminium chloride he...	12047512	3
Fagron	Aluminium chloride he...	12/27-n01	1
Fagron	Aluminium potassium s...	A1-063-A1	1
Fagron	Aluminium potassium s...	13D29-N04	1
Fagron	Aluminium potassium s...	103638	1
Fagron	Aluminium potassium s...	13D08-N01	1
Fagron	Aluminium potassium s...	12/24-M02	1
Fagron	Aluminium potassium s...	A1-063-AL	1
Fagron	Aluminium potassium s...	12I24-M03	1
Fagron	Amphetamine sulfate	13D09-N03	1
Fagron	Amphetamine sulfate	16A29-B03-324578	2
Fagron	Amphetamine sulfate	16A29-B03-328317	3
Fagron	Amphetamine sulfate	13B11-N04	2
Fagron	Amphetamine sulfate	16K08-B04-336361	1
Fagron	Amphetamine sulfate	13G08-N11	3
Fagron	Amphetamine sulfate	11D04-N13	1
Fagron	Amphetamine sulfate	12B06-N13	2
Fagron	Amphetamine sulfate	12E11-N06	2
Fagron	Amphetamine sulfate	11/01-N01	1
Fagron	Amphetamine sulfate	17K03-B01-344122	1
Fagron	Amphetamine sulfate	315291	1
Fagron	Amphetamine sulfate	13J18-B40-290538	1
Fagron	Amphetamine sulfate	96200	1
Fagron	Amphetamine sulfate	13J18-B40	1
Fagron	Amphetamine sulfate	78012	1
Fagron	Amphetamine sulfate	324577	2
Fagron	Amphetamine sulfate	12/24N-03	1
Fagron	Amphetamine sulfate	88689	2
Fagron	Amphetamine sulfate	14E19-B09	2
Fagron	Amphetamine sulfate	14E19-B09-294572	1
Fagron	Amphetamine sulfate	13J18B40	1
Fagron	Amphetamine sulfate	14E19-B09-304502	2
Fagron	Amphetamine sulfate	15L01-B05-315291	3
Fagron	Amphetamine sulfate	2213Q-03361	1
Fagron	Amphetamine sulfate	16A29-B03	8
Fagron	Amphetamine sulfate	16A29-B03-318743	6
Fagron	Amphetamine sulfate	15101-b05-315292	1
Fagron	Aniseed	11370304	6
Fagron	Barbital sodium	15L07-B02	1

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Supplier	Substance	Batch	Spectra
Fagron	Betaine hydrochloride	15121401	1
Fagron	Betaine hydrochloride	12C20-N09	1
Fagron	Betaine hydrochloride	24091301	1
Fagron	Betaine hydrochloride	13G29-B02-294870	1
Fagron	Betamethasone-17-vale...	13E08-N01	1
Fagron	Betamethasone-17-vale...	12G02-N02	2
Fagron	Betamethasone-17-vale...	12J19-N06	1
Fagron	Betamethasone-17-vale...	12L19-N06	4
Fagron	Betamethasone-17-vale...	12G02-N15	3
Fagron	Betamethasone-17-vale...	12C19-N07	1
Fagron	Birch leaf, cut	7061301	1
Fagron	Bitter fennel	1406211545	1
Fagron	Bitter fennel	6858913	1
Fagron	Bitter fennel		1
Fagron	Caffeine citrate	15A05-B03-318006	12
Fagron	Caffeine citrate	15a05-b03-318006	1
Fagron	Caffeine citrate	2002311282	1
Fagron	Caffeine citrate	15A05B03	1
Fagron	Caffeine citrate	15A05-B03	3
Fagron	Caffeine citrate	15A05-B03	1
Fagron	Caffeine citrate	11C29-N04	1
Fagron	Caffeine citrate	13D30-N02	1
Fagron	Caffeine citrate	2714E-01282	1
Fagron	Caffeine citrate	3314E-01282	1
Fagron	Caffeine citrate	11082015A	1
Fagron	Caffeine citrate	CCC1205	1
Fagron	Caffeine citrate	13D30-No2	1
Fagron	Caffeine citrate	5013U01282	1
Fagron	Caffeine citrate	4213U01282	1
Fagron	Caffeine citrate	3513I-01282	1
Fagron	Caffeine citrate	12C16-N03	1
Fagron	Caffeine citrate	2813E1282	1
Fagron	Caffeine citrate	10H02-N02	2
Fagron	Caffeine citrate	26021401	1
Fagron	Caffeine citrate	15A05-B03-307135	3
Fagron	Caffeine citrate	CCD-1401	3
Fagron	Caffeine citrate	15a05-b03-302746	1
Fagron	Caffeine citrate	11C29-N04	1
Fagron	Caffeine citrate	204311282	1
Fagron	Caffeine citrate	3914U-01282	1
Fagron	Caffeine citrate	12J05-N06	1
Fagron	Calendula flower, cut	1241B120312	3
Fagron	Chlorhexidine dihydro...	14A09-B03-293425	1
Fagron	Cinchocaine hydrochlo...	12F25-N10	1
Fagron	Cinnarizine	13I26-N22	1
Fagron	Cinnarizine	13I26-N22	1
Fagron	Cinnarizine	8D11-N04	1
Fagron	Cinnarizine	14D09-B01	3
Fagron	Cinnarizine	14D09-B01-292883	1
Fagron	Cinnarizine	13H01-N07	4
Fagron	Clobetasol-17-propion...	12/19-No1	1
Fagron	Clobetasol-17-propion...	12/19-N01003637	1
Fagron	Clobetasol-17-propion...	12/19-N01	1
Fagron	Clobetasol-17-propion...	12I19-N01	1
Fagron	Clobetasol-17-propion...	12I19-N01	1
Fagron	Clobetasol-17-propion...	13W16-N01	1
Fagron	Clobetasol-17-propion...	12L19-N06	1
Fagron	Clobetasol-17-propion...	12K08-N02	2
Fagron	Cocaine hydrochloride	15-00638	1
Fagron	Cocaine hydrochloride	15E12-B03	1

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Supplier	Substance	Batch	Spectra
Fagron	Cocaine hydrochloride	14H27-B03	1
Fagron	Cocaine hydrochloride	12G23-N13	1
Fagron	Cocaine hydrochloride	16B11-B05-323385	1
Fagron	Codeine phosphate hem...	13E21-N04	1
Fagron	Codeine phosphate hem...	15B17-B99-304623	1
Fagron	Codeine phosphate hem...	13/27-N06	2
Fagron	Codeine phosphate hem...	15F09-B02-310520	2
Fagron	Codeine phosphate hem...	13C11-N10	1
Fagron	Codeine phosphate hem...	1615I-01279	1
Fagron	Codeine phosphate hem...	15F09-B02-314033	1
Fagron	Codeine phosphate hem...	15F09-B02	1
Fagron	Codeine phosphate hem...	913I-01279	1
Fagron	Codeine phosphate hem...	16E17-B05-324109	4
Fagron	Codeine phosphate hem...	12C05-N01	1
Fagron	Codeine phosphate hem...	11/19-N10	1
Fagron	Copper (II) sulfate p...	13A25-N06	1
Fagron	Deoxycholic acid	13J21-N14	1
Fagron	Dexamethasone 1:10 (r...	12C20-N03	4
Fagron	Dexamethasone 1:10 (r...	12K06-N09	1
Fagron	Dexamethasone 1:10 (r...	12L19-N06	1
Fagron	Dexamphetamine sulfate	15H06-B04-313861	1
Fagron	Dexamphetamine sulfate	17B09-B02-339689	1
Fagron	Dexamphetamine sulfate	11F29-N01	1
Fagron	Dexamphetamine sulfate	17B09-B02-339690	1
Fagron	Dihydrocodeine hydrog...	15F18-B07-323388	1
Fagron	Dihydrocodeine hydrog...	14K26-B04	1
Fagron	Dihydrocodeine hydrog...	17G04-B02-342861	1
Fagron	Dihydrocodeine hydrog...	16I27-B03-332122	1
Fagron	Dihydrocodeine hydrog...	14D08-B06	1
Fagron	Dihydrocodeine hydrog...	13H19-N08	3
Fagron	Dihydrocodeine hydrog...	12G05-N01	1
Fagron	Dihydrocodeine hydrog...	14K26-B04-310974	1
Fagron	Econazole nitrate	11F09-N16	1
Fagron	Econazole nitrate	14G22-B07-306926	1
Fagron	Econazole nitrate	13D22-N06	1
Fagron	Fentanyl citrate	20100911-1	1
Fagron	Fentanyl citrate	10H20-N02	1
Fagron	Fenugreek, powdered	12149603	1
Fagron	Frankincense		1
Fagron	Fuchsine	12A03-N06	1
Fagron	Fuchsine	12G18-N01	1
Fagron	Fuchsine	12F28-N02	1
Fagron	Fuchsine	13A30-N05	1
Fagron	Fuchsine	13H23-M04	2
Fagron	Heavy alkaline bismut...	13H28-B04-291385	1
Fagron	Heavy alkaline bismut...	11/13-N01	1
Fagron	Heavy alkaline bismut...	13B25-N02	3
Fagron	Heavy alkaline bismut...	1001311186	1
Fagron	Heavy alkaline bismut...	1309211186	1
Fagron	Heavy alkaline bismut...	12C08-N06	3
Fagron	Heavy alkaline bismut...	11D28-N16	1
Fagron	Heavy alkaline bismut...	12D26-N03	1
Fagron	Heavy alkaline bismut...	13C15-N05	3
Fagron	Hydromorphone hydroch...	12G05-N02	1
Fagron	Indigo carmine	11F09-N06	1
Fagron	Indigo carmine	12A20-N067-16	1
Fagron	Indigo carmine	12K06-N11	1
Fagron	Ladys bedstraw herb,...	12369004	2
Fagron	Lavender flower	1489A120919	6
Fagron	Lungwort herb, cut	Nachprüfung	1

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Supplier	Substance	Batch	Spectra
Fagron	Macrogols 6000 powder	14J17-B01	1
Fagron	Macrogols 6000 powder	11G14-N03	1
Fagron	Macrogols 6000 powder	12J22-N02	1
Fagron	Magnesium aspartate d...	17C21-B05-333111	1
Fagron	Magnesium carbonate, ...	12F20-N04	1
Fagron	Magnesium chloride he...	1304C003	1
Fagron	Magnesium chloride he...	1301C10-277801	1
Fagron	Magnesium chloride he...	1301C10	3
Fagron	Magnesium chloride he...	12h21-N02	1
Fagron	Magnesium chloride he...	1301C009-277802	4
Fagron	Magnesium chloride he...	1301C011-277803	1
Fagron	Magnesium chloride he...	M1625	1
Fagron	Magnesium chloride he...	M1555	1
Fagron	Magnesium chloride he...	12H21-N02	1
Fagron	Magnesium chloride he...	1301C012-277804	1
Fagron	Magnesium chloride he...	1304C002	1
Fagron	Magnesium chloride he...	1304c004-281210	1
Fagron	Magnesium chloride he...	26061305	1
Fagron	Magnesium chloride he...	1301c009-277802	1
Fagron	Magnesium chloride he...	1304C001-281211	2
Fagron	Magnesium chloride he...	1304C003-281209	1
Fagron	Magnesium chloride he...	13411207	1
Fagron	Magnesium chloride he...	13B14-B01-287292	1
Fagron	Magnesium chloride he...	M1430	1
Fagron	Magnesium chloride he...	11K17-N10	1
Fagron	Magnesium chloride he...	12H21-N02	9
Fagron	Magnesium chloride he...	12B16-N01	1
Fagron	Magnesium chloride he...	1304C004-281210	1
Fagron	Magnesium chloride he...	12H21-No2	1
Fagron	Magnesium chloride he...	12D11-N01	1
Fagron	Magnesium sulfate hep...	12L10-N07	1
Fagron	Magnesium sulfate hep...	12G24-N02	1
Fagron	Magnesium sulfate hep...	31161	1
Fagron	Magnesium sulfate hep...	12L10-N07	8
Fagron	Magnesium sulfate hep...	26251	1
Fagron	Magnesium sulfate hep...	13H05-N02	1
Fagron	Matricaria flower		1
Fagron	Methadone hydrochloride	12H07-N07	1
Fagron	Methadone hydrochloride	17/15-B02-343153	1
Fagron	Methadone hydrochloride	8081501	1
Fagron	Methadone hydrochloride	1409H043	1
Fagron	Methadone hydrochloride	15B24-B02-304724	6
Fagron	Methadone hydrochloride	29051502	1
Fagron	Methadone hydrochloride	18C01B05350571	1
Fagron	Methadone hydrochloride	4031517	1
Fagron	Methadone hydrochloride	14C24-B01-292857	4
Fagron	Methadone hydrochloride	13J24-B06-286908	1
Fagron	Methadone hydrochloride	1327h051	1
Fagron	Methadone hydrochloride	13J24-B06-286907	1
Fagron	Methadone hydrochloride	25091406	1
Fagron	Methadone hydrochloride	13I24-B06-286908	1
Fagron	Methadone hydrochloride	11D07-N09	1
Fagron	Methadone hydrochloride	1437H012	2
Fagron	Methadone hydrochloride	1316H037	4
Fagron	Methadone hydrochloride	11G11-N02	1
Fagron	Methadone hydrochloride	25091307	1
Fagron	Methadone hydrochloride	13F17-N02	6
Fagron	Methadone hydrochloride	12b21-n03	1
Fagron	Methadone hydrochloride	12B21N03	1
Fagron	Methadone hydrochloride	13B06-N02	5

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Supplier	Substance	Batch	Spectra
Fagron	Methadone hydrochloride	1225H008	1
Fagron	Methadone hydrochloride	12A05-No2	1
Fagron	Methadone hydrochloride	171920-0009	1
Fagron	Methadone hydrochloride	9041306	1
Fagron	Methadone hydrochloride	1213E-02949	1
Fagron	Methadone hydrochloride	12H07-N05	4
Fagron	Methadone hydrochloride	20130912-6	1
Fagron	Methadone hydrochloride	414022-1-P	1
Fagron	Methadone hydrochloride	14H15-B01	1
Fagron	Methadone hydrochloride	14H15-B01-299381	1
Fagron	Methadone hydrochloride	15E29-B02-309070	2
Fagron	Methadone hydrochloride	17I15-B02-343153	1
Fagron	Methadone hydrochloride	17I15-B02	2
Fagron	Methadone hydrochloride	17I15-B02-339521	1
Fagron	Methadone hydrochloride	17I15W02	1
Fagron	Methadone hydrochloride	1718H028	3
Fagron	Methadone hydrochloride	17c24b05334309	1
Fagron	Methadone hydrochloride	17C24-B05-335711	7
Fagron	Methadone hydrochloride	17I15-B02-339529	2
Fagron	Methadone hydrochloride	14H15-B01-299382	6
Fagron	Methadone hydrochloride	16-k01-B04-329937	1
Fagron	Methadone hydrochloride	17C24-B05-334309	2
Fagron	Methadone hydrochloride	16f24-b02-323184	1
Fagron	Methadone hydrochloride	16F24B02323184	2
Fagron	Methadone hydrochloride	16K01-B04	1
Fagron	Methadone hydrochloride	16F24-B02-329935	1
Fagron	Methadone hydrochloride	16B16-Bo2	1
Fagron	Methadone hydrochloride	16K01-B04-329934	1
Fagron	Methadone hydrochloride	15E29-B02-313098	3
Fagron	Methadone hydrochloride	15B24-B02-313097	1
Fagron	Methadone hydrochloride	16B16-B02-318420	2
Fagron	Methadone hydrochloride	15I24-B07	1
Fagron	Methadone hydrochloride	1514H042	2
Fagron	Methadone hydrochloride	13J24B06286910	1
Fagron	Methadone hydrochloride	16F24-B02-323182	1
Fagron	Methadone hydrochloride	16F24-B02-323185	1
Fagron	Methadone hydrochloride	16F24-B02-326207	2
Fagron	Methadone hydrochloride	170427MH/1608H002	1
Fagron	Methadone hydrochloride	15E29_B02_309070	1
Fagron	Methadone hydrochloride	16F24-B02-323186	1
Fagron	Methadone hydrochloride	1608H002	2
Fagron	Methylrosanilinium ch...	13H28-N03	2
Fagron	Methylrosanilinium ch...	13H28-N03-0161-1030	1
Fagron	Methylrosanilinium ch...	13H28-No3	1
Fagron	Methylrosanilinium ch...	12D19-N01	1
Fagron	Methylrosanilinium ch...	12I17-N05	1
Fagron	Methylrosanilinium ch...	13G03N11	1
Fagron	Methylrosanilinium ch...	13H28-N03	18
Fagron	Methylrosanilinium ch...	13G03-N11	1
Fagron	Methylrosanilinium ch...	12H28_N06	1
Fagron	Methylrosanilinium ch...	13G03-N011	1
Fagron	Methylrosanilinium ch...	13H28-N03	1
Fagron	Methylrosanilinium ch...	12-17-N050109-140	1
Fagron	Midazolam	16J03-B09-326963	1
Fagron	Midazolam	14C12-B31-313222	1
Fagron	Midazolam hydrochloride	400101	1
Fagron	Midazolam hydrochloride	9D27-N01	2
Fagron	Midazolam hydrochloride	11A31-N01	1
Fagron	Midazolam hydrochloride	15H04-B03-314396	6
Fagron	Midazolam hydrochloride	14H05-B08-297982	1

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Supplier	Substance	Batch	Spectra
Fagron	Morphine hydrochloride	17C24-B03-334287	1
Fagron	Morphine hydrochloride	16D21-B02-322087	1
Fagron	Morphine hydrochloride	15J27_B01_316889	1
Fagron	Morphine hydrochloride	15I09-B08-312693	1
Fagron	Morphine hydrochloride	15A12-B04-303137	1
Fagron	Morphine hydrochloride	12E10-N04	2
Fagron	Morphine hydrochloride	13H22-N12	1
Fagron	Morphine hydrochloride	12E10N04	1
Fagron	Morphine hydrochloride	11A27-N04	1
Fagron	Morphine hydrochloride	13D09-N04	1
Fagron	Nitrofurantoin	15J15-B06	2
Fagron	Nitrofurantoin	15J15-B06-317250	2
Fagron	Nitrofurantoin	12C30-N03	1
Fagron	Nitrofurantoin	11F07-N06	3
Fagron	Nitrofurantoin	13D10-N03	1
Fagron	Nitrofurantoin	15J15-B06-313939	1
Fagron	Nitrofurantoin	13A08-N01	1
Fagron	Nitrofurantoin	3071403	1
Fagron	Nitrofurantoin	15J15-B06-319031	1
Fagron	Nitrofurantoin	15J15-B06-315225	2
Fagron	Nitrofurantoin	201203080296	1
Fagron	Nitrofurantoin	2714I-03527	1
Fagron	Nitrofurantoin	13B28-N07	1
Fagron	Nitrofurantoin	71/14	1
Fagron	Orris root	11026705	3
Fagron	Peppermint leaf, cut	13030803	3
Fagron	Peppermint leaf, cut	1234567	2
Fagron	Phenobarbital	13G05-N09	1
Fagron	Phenobarbital	15G07-B06-311718	1
Fagron	Potassium hydrocarbon...	12K27-N06	1
Fagron	Potassium hydrocarbon...	13031205	1
Fagron	Potassium hydrocarbon...	120801001	1
Fagron	Potassium hydrocarbon...	12141911	1
Fagron	Prednisolone 1:10 (ri...	12D04-N01	1
Fagron	Prednisolone 1:10 (ri...	12L19-N06	1
Fagron	Rhubarb, powdered	11043821	1
Fagron	Rutoside trihydrate	13K12-B06	1
Fagron	Rutoside trihydrate	L14050127	1
Fagron	Saffron filaments	380A120416	1
Fagron	Senna leaf, cut	314Q1514	1
Fagron	Sodium alginate	14G22-B99	1
Fagron	Sodium dihydrogen pho...	12L05-N05	1
Fagron	Sodium hydrogen carbo...	13G11-N03	2
Fagron	Sodium hydrogen carbo...	4413I01892	1
Fagron	Sodium hydrogen carbo...	13B18-N03	6
Fagron	Sodium hydrogen carbo...	13D29-N09	4
Fagron	Sodium hydrogen carbo...	12D11-No2	1
Fagron	Sodium hydrogen carbo...	RBA3651200	1
Fagron	Sodium hydrogen carbo...	RBA3421100	3
Fagron	Sodium hydrogen carbo...	12G11-N03	7
Fagron	Sodium hydrogen carbo...	11K25-N05	3
Fagron	Sodium hydrogen carbo...	11/12-N16	1
Fagron	Sodium hydrogen carbo...	11I12-N16	3
Fagron	Sodium hydrogen carbo...	12D11-N02	9
Fagron	Sodium hydroxide pell...	13F06-N02	3
Fagron	Sodium hydroxide pell...	12E02-N15	1
Fagron	Sodium hydroxide pell...	13k22-no5	1
Fagron	Sodium monohydrogenph...	13D24-N12	2
Fagron	Sodium monohydrogenph...	613I-01914	1
Fagron	Sodium monohydrogenph...	13H01-B01	1

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Supplier	Substance	Batch	Spectra
Fagron	Sodium monohydrogenph...	11K30-N01	1
Fagron	Sodium monohydrogenph...	1513I-01914	1
Fagron	Sodium monohydrogenph...	B44888A	1
Fagron	Sodium monohydrogenph...	2111E-01914	1
Fagron	Sodium sulfate decahy...	1464	1
Fagron	Sodium sulfate decahy...	2134	1
Fagron	Sodium thiosulfate pe...	13092013E	1
Fagron	Sodium thiosulfate pe...	3313U-01922	1
Fagron	Sodium thiosulfate pe...	12F20-N10	1
Fagron	Sodium thiosulfate pe...	12F20-N20	1
Fagron	Sulfanilamide	11L01-No8	1
Fagron	Sweet fennel	2870A130304	3
Fagron	Thiomersal	12J17-N02	1
Fagron	Thiomersal	12J17-N02	1
Fagron	Thiomersal	12F19-N11	1
Fagron	Triamcinolone acetoni...	12A05-N07	3
Fagron	Triamcinolone acetoni...	11G14-N02	1
Fagron	Triamcinolone acetoni...	13A15-N05	1
Fagron	Triamcinolone acetoni...	13F21-N01	2
Fagron	Triamcinolone acetoni...	13F20-N010113/150	1
Fagron	Triamcinolone acetoni...	12F21-N01	1
Fagron	Triamcinolone acetoni...	12I07-N04	1
Fagron	Triamcinolone acetoni...	12E23-N01	2
Fagron	Triamcinolone acetoni...	12I07-N04	1
Fagron	Triamcinolone acetoni...	12G23-N06	2
Fagron	Triamcinolone acetoni...	12I07-No4	1
Fagron	Triamcinolone acetoni...	14F17-N02	1
Fagron	Triamcinolone acetoni...	12I07-N04022/359	1
Fagron	Trichloroacetic acid	13B19-M04	1
Fagron	Trichloroacetic acid	13H22-M04	1
Fagron	Wild pansy, cut		1
Fagron	Yarrow herb, cut	3613M-0165	1
Falcento	D-(+)-mannose	R-4639	1
Falcento	D-(+)-mannose	R4640	1
Falcento	D-(+)-mannose	R-4641	1
Falcento	D-(+)-mannose	R-4638	1
Falcento	D-ribose	JXCZSJ14-D-010	1
Falcento	D-ribose	201206712	2
Falcento	D-ribose	201209702	1
fargon	Magnesium sulfate hep...	12E22-N02	4
Fargon	Caffeine citrate	12J05-N06	4
Fargon	Methadone hydrochloride	16K01-B04-329937	2
Fargon / Gehe	Cinnamon, cut	15104201	1
Fargon/17.07.2013/Now...	Triamcinolone acetoni...	12I07-N04	1
Fargon/Gehe	Dexamphetamine sulfate	15H06-B04	1
Fargon/Phoenix	Caffeine citrate	15A05-B03-302746	11
fargon/Sanacorp	Sodium sulfate decahy...	12H31-N04	1
Fargon/Noweda	Sweet fennel	2870A150810	1
Faron	Aluminium chloride he...	13I13-B03-287298	1
Fgron	Caffeine citrate	2013Q-01282	1
Fgron GmbH & Co. KG	Methadone hydrochloride	18C01-B05-350571	1
Fiebig 05.11.12 ek:9...	Bilberry fruit, dried	2910A120410	1
Fiebig 16.11.12 ek:2,35	Walnut bark, cut	711B111020	5
Fiebig ek:9.84EUR 24.09...	Peppermint leaf, cut	2181A110512	5
Finze	Centaury, cut	11097610	1
Finze	Elder flower, rubbed	9297415	1
Finze	Equisetum stem, cut	11076305	8
Finze	Frangula bark, cut	249091	1
Finze	Knotgrass, cut	10237202	1
Finze	Linseed	3607E-02240	1

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Supplier	Substance	Batch	Spectra
Finze	Lycopodium herb, cut	9378803	1
Finze	Male speedwell wort, ...	4661B080915	1
Finze	Matricaria flower	12361703	6
Finze	Matricaria flower	1290B101122	1
Finze	Sage leaf, cut	2301A110204	7
Finze	Sodium hydrogen carbo...	Pr.Nr.4311Q-01892	1
Finze	St. John's wort, cut	9297303	1
Finze	Wild thyme, cut	11031204	1
fischar	Sodium hydrogen carbo...	6522101	6
Fischer/VDL	Sodium hydrogen carbo...	6521111	5
Gahlke	Aniseed, pounded	21401	1
Gahlke	Bitter fennel	20362	1
Gahlke	Frankincense	21949	1
Gahlke	Parsley root, cut	20872	1
Gahlke	Sorrel herb, cut	21479	1
Gahlke	Sweet woodruff herb, ...	22100	1
galke	Aniseed	19654	1
galke	Bitter fennel	19938	3
galke	Melissa leaf, cut	20867	1
Galke	Acorus root, peeled	18944	1
Galke	Agrimony, cut	2002	1
Galke	Alchemilla, cut	22291	1
Galke	Alchemilla, cut	21141	1
Galke	Alchemilla, cut	19835	1
Galke	Aniseed	23464	1
Galke	Aniseed	21278	1
Galke	Aniseed	22274	1
Galke	Asparagus root, cut	20178	1
Galke	Bean shells, cut	21219	1
Galke	Bearberry leaf, cut	19936	3
Galke	Birch leaf, cut	21226	1
Galke	Birch leaf, cut	20904	1
Galke	Bitter fennel	22176	1
Galke	Blackcurrants	21348	1
Galke	Blue bottle flower wi...	23131	2
Galke	Boldo leaf, cut	19855	1
Galke	Burdock root, cut	19802	1
Galke	Caraway fruit	23627	1
Galke	Caraway fruit	27450	1
Galke	Caraway fruit	21257	1
Galke	Caraway fruit, pounded	18943	1
Galke	Centaury, cut	9721	1
Galke	Chelidonium majus her...	20937	3
Galke	Common broom herb, cut	12358803	4
Galke	Common wormwood herb,...	21637	1
Galke	Couch grass rhizome, ...	18781	1
Galke	Dandelion herb with r...	22093	2
Galke	Dandelion herb with r...	20531	6
Galke	Dandelion root, cut	126302	1
Galke	Dandelion root, cut	20658	1
Galke	Devil's claw root	20282	2
Galke	Devil's claw root	21018	2
Galke	Dill fruit	22422	4
Galke	Elder flower, rubbed	21934	1
Galke	Elecampane rhizome, cut	21569	2
Galke	Equisetum stem, cut	19663	5
Galke	Equisetum stem, cut	22061	1
Galke	Euphrasy herb, cut	20262	2
Galke	Gentian root, cut	19192	2
Galke	Geum urbanum herb, cut	20881	1

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Supplier	Substance	Batch	Spectra
Galke	Ginger, peeled	21766	2
Galke	Ginger, peeled	20633	1
Galke	Goat's rue, cut	8378	2
Galke	Hawthorn leaf with fl. ...	21126	3
Galke	Hay flower	21926	1
Galke	Hop strobile	23363	1
Galke	Hop strobile	20928	2
Galke	Hop strobile	20928	3
Galke	Horse chestnut flower. ...	2614	1
Galke	Hyssop herb, cut	20939	1
Galke	Iceland moss, cut	12369	1
Galke	Ladys bedstraw herb, ...	21942	2
Galke	Lavender flower	21416	2
Galke	Lemon peel, cut	22975	1
Galke	Liquorice root, peeled	23538	1
Galke	Lungwort herb, cut	19511	4
Galke	Lycopodium herb, cut	16913	3
Galke	Mallow flower, cut	21119	1
Galke	Mallow leaf, cut	21454	1
Galke	Mallow leaf, cut	21445	1
Galke	Mallow leaf, cut	17133	1
Galke	Manna, powdered	20669	1
Galke	Manna, powdered	19784	1
Galke	Marian thistle fruit	22187	4
Galke	Marjoram herb, rubbed	23241	1
Galke	Marjoram herb, rubbed	22401	1
Galke	Masterwort root, cut	18411	1
Galke	Masterwort root, cut	23074	1
Galke	Maté leaf, cut	22365	1
Galke	Matricaria flower	18803	1
Galke	Matricaria flower	21652	1
Galke	Matricaria flower	18471	5
Galke	Meadowsweet herb, cut	20358	1
Galke	Mistletoe, cut	22012	2
Galke	Mistletoe, cut	20328	1
Galke	Nettle leaf, cut	21238	1
Galke	Nettle leaf, cut	20956	1
Galke	Nettle leaf, cut	23302	1
Galke	Nutmeg, powdered (spi. ...)	22739	1
Galke	Oak bark, cut	17824	2
Galke	Orris root	21303	1
Galke	Peppermint leaf, cut	22218	1
Galke	Peppermint leaf, cut	20975	3
Galke	Peppermint leaf, cut	22783	3
Galke	Primrose flower	22612	2
Galke	Psyllium seed	22989	7
Galke	Psyllium seed	20968	2
Galke	Raspberry leaf, cut	21244	1
Galke	Raspberry leaf, cut	23532	1
Galke	Raspberry leaf, cut	18060	2
Galke	Raspberry leaf, cut	19499	2
Galke	Red clover flower	23128	2
Galke	Red-rose petal	22641	2
Galke	Restharrow root, cut	12700	1
Galke	Ribwort plantain, cut	21598	1
Galke	Ribwort plantain, cut	20259	1
Galke	Rosemary leaf, cut	22777	1
Galke	Rosemary leaf, cut	19813	1
Galke	Rosemary leaf, cut	21390	1
Galke	Sage leaf, cut	21015	3

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Supplier	Substance	Batch	Spectra
Galke	Sanicle herb, cut	23097	1
Galke	Senna leaf, cut	21778	1
Galke	Shepherd's purse, cut	21719	2
Galke	Shepherd's purse, cut	19483	1
Galke	Silverweed, cut	12891	2
Galke	St. John's wort, cut	21034	1
Galke	St. John's wort, cut	21990	4
Galke	St. John's wort, cut	21556	1
Galke	St. John's wort, cut	23054	1
Galke	Tall golden rod, cut	21079	2
Galke	Thyme, rubbed	20719	2
Galke	Thyme, rubbed	1833	1
Galke	Thyme, rubbed	19386	2
Galke	Thyme, rubbed	28719	1
Galke	Tormentil	21744	2
Galke	Tormentil	21091	1
Galke	Turmeric root, cut	20184	1
Galke	Turmeric root, cut	23123	1
Galke	Turmeric, javanese, cut	15540	1
Galke	Turmeric, javanese, cut	15540	1
Galke	Valerian root, cut	22070	1
Galke	Valerian root, cut	21798	4
Galke	Walnut leaf, cut	21061	1
Galke	White deadnettle flower	22704	1
Galke	White deadnettle flower	21691	4
Galke	White deadnettle herb...	19706	1
Galke	White deadnettle herb...	22253	2
Galke	Willow bark, cut	20338	1
Galke	Willowherb, small flo...	22347	4
Galke	Willowherb, small flo...	47502	1
Galke	Wormwood herb, cut	21330	1
Galke	Yarrow herb, cut	23318	1
Galke	Yarrow herb, cut	22048	7
Galke	Yarrow herb, cut	21295	2
Galke	Yarrow herb, cut	23735	1
galke,	Calendula flower	12028	1
galke,	Lime flower, cut	2098	1
gasser	Angelica root	950049	1
Gatt Koller/Herba	Amphetamine sulfate	942/03130814	1
Gatt-Koller	Betaine hydrochloride	2970/07102910	1
gebepharm	Sodium monohydrogenph...	20160909-2	1
gehe	Methadone hydrochloride	16135316	3
Gehe	Acorus root, peeled	6701B130807	9
Gehe	Alchemilla, cut	1341102	1
Gehe	Aluminium chloride he...	12114902	3
Gehe	Aluminium chloride he...	130701102	1
Gehe	Angelica root	285732	1
Gehe	Aniseed	10247203	1
Gehe	Aniseed, pounded	13149903	1
Gehe	Arnica flower	11259801	2
Gehe	Bitter fennel	2860A120412	23
Gehe	Blackberry leaf, cut	10136409	1
Gehe	Caffeine citrate	13B08-N02	3
Gehe	Calendula flower, cut	260205	1
Gehe	Codeine phosphate hem...	15350710	2
Gehe	Coltsfoot leaf, cut	2021B121204	9
Gehe	Couch grass rhizome, ...	12186704	1
Gehe	Couch grass rhizome, ...	283061	1
Gehe	Dandelion herb with r...	6611B110104	1
Gehe	Dandelion herb with r...	13019803	1

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Supplier	Substance	Batch	Spectra
Gehe	Deoxycholic acid	2012060253	1
Gehe	Devil's claw root	1114005	1
Gehe	Elder berries	12267807	1
Gehe	Elder flower, rubbed	1090413	1
Gehe	Elder flower, rubbed	1250213	1
Gehe	Elecampane rhizome, cut	11196906	1
Gehe	Elecampane rhizome, cut	12113302	2
Gehe	Equisetum stem, cut	11076301	4
Gehe	Equisetum stem, cut	10375515	1
Gehe	Equisetum stem, cut	12288803	13
Gehe	Fenugreek	13013811	2
Gehe	Fenugreek	11313204	1
Gehe	Frangula bark, cut	11254003	2
Gehe	Frangula bark, cut	11254004	4
Gehe	Frangula bark, cut	11254006	4
Gehe	Fumitory, cut	12103402	2
Gehe	Galeopsis herb, cut	3911A130320	6
Gehe	Hawthorn leaf with fl. ...	1351B111207	2
Gehe	Horse chestnut leaf, ...	2551B131024	1
Gehe	Iceland moss, cut	11053915	1
Gehe	Iceland moss, cut	11101603	1
Gehe	Ivy leaf, cut	2061B080402	1
Gehe	Juniper, pounded	13020903	1
Gehe	Kaolin, heavy	11350107	3
Gehe	Liquorice root, peeled	1250213	1
Gehe	Liquorice root, peeled	270853	3
Gehe	Liquorice root, peeled	268835	1
Gehe	Liquorice root, natur. ...	277004	2
Gehe	Liquorice root, natur. ...	283316	1
Gehe	Liquorice root, natur. ...	284243	2
Gehe	Mallow flower, cut	1501B120508	6
Gehe	Mallow flower, cut	1501B110207	1
Gehe	Mallow leaf, cut	2131B110420	2
Gehe	Mallow leaf, cut	10290512	1
Gehe	Marian thistle herb, ...	10365602	2
Gehe	Marshmallow root, pee. ...	6071A120306	2
Gehe	Matricaria flower	12133009	1
Gehe	Matricaria flower	11214802	1
Gehe	Matricaria flower	12337605	1
Gehe	Matricaria flower	11255204	1
Gehe	Melilot herb, cut	110324	1
Gehe	Melissa leaf, cut	12032314	4
Gehe	Motherwort herb, cut	12231502	3
Gehe	Nettle leaf, cut	10162701	1
Gehe	Nettle leaf, cut	2381A120619	13
Gehe	Nettle root, cut	6631B120927	5
Gehe	Parsley root, cut	6441A110210	3
Gehe	Peppermint leaf, cut	2181B130717A	1
Gehe	Peppermint leaf, cut	2181B130717B	1
Gehe	Primrose flower	11374401	1
Gehe	Rhubarb, cut	13235208	2
Gehe	Ribwort plantain, cut	1080413	1
Gehe	Rue herb, cut	12148802	1
Gehe	Silverweed, cut	11328101	1
Gehe	Sodium hydrogen carbo...	1203030-02	8
Gehe	Sodium hydrogen carbo...	12k09-N05	1
Gehe	Sodium hydrogen carbo...	11078315	1
Gehe	Sodium monohydrogenph...	12109001	2
Gehe	Sodium sulfate decahy...	12257902	6
Gehe	St. John's wort, cut	11185602	1

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Supplier	Substance	Batch	Spectra
Gehe	St. John's wort, cut	9297305	1
Gehe	Tall golden rod, cut	11207011	1
Gehe	Tall golden rod, cut	11280311	2
Gehe	Thyme, rubbed	4622A110120	1
Gehe	Verbena herb, cut	4651B110310	2
Gehe	Walnut bark, cut	711B110128	3
Gehe	Walnut leaf, cut	2111B151028	2
Gehe	Walnut leaf, cut	10050412	1
Gehe	Wild pansy, cut	11216103	3
Gehe	Wild thyme, cut	1090413	1
Gehe	Wormwood herb, cut	11285811	1
Gehe	Wormwood herb, cut	13381901	1
Gehe	Yarrow herb, cut	1128503	1
Gehe	Yarrow herb, cut	4181A111122	5
Gehe	Yarrow herb, cut	279023	3
Gehe / 08.03.13 Redwood	Blessed thistle, cut	205007	1
gehe 07.12.2013	Sage leaf, cut	2301/7120403	1
GEHE 10.03.2014	Oak bark, cut	761A11816	1
gehe 10.12.13	Raspberry leaf, cut	229117121120	1
GEHE 21.10.2014	Deoxycholic acid	13F13-N06	1
Gehe am 27.03.2014	Juniper, pounded	2890A130513	1
Gehe/Noweda	Methadone hydrochloride	16135319	2
Gesundform	Mistletoe, cut	216482	1
Giusto Faravelli	D-(+)-mannose	161004/1710215001	1
Gutenberg-Apotheke	Agnus castus fruit	61765	1
Gutenberg-Apotheke	Aniseed	1333902	1
Gutenberg-Apotheke	Ground ivy herb, cut	11374610	3
Gutenberg-Apotheke	Nettle leaf, cut	18897	1
Gutenberg-Apotheke	Oak bark, cut	11351206	13
Gutenberg-Apotheke	Raspberry leaf, cut	28911	1
Haustee	Mistletoe, cut	57010507	1
HBK Gesundheit	Maltodextrin	1143	3
HBK Gesundheit	Maltodextrin	2343	1
Hedinger	Dandelion herb with r...	10121614	1
Hedinger	Dihydrocodeine hydrog...	70162	4
Hedinger	Linseed	16011402	1
Hedinger	Magnesium sulfate hep...	204037	2
Hedinger	Rhubarb, powdered	13193110	1
Hedinger/ Sanacorp	Methadone hydrochloride	15215505	3
Hedinger/Phönix	Sodium sulfate decahy...	205025	1
Heinrich Kle/Sanacor	Linseed	7307A170111	2
Hepart AG	Alchemilla, cut	B-698kbA	1
Hepart AG	Alchemilla, cut	21963	3
Hepart AG	Aniseed	B216346, kbA	1
Hepart AG	Bitter fennel	B492, kbA	1
Hepart AG	Bitter orange flower ...	B120822	1
Hepart AG	Black cumin seed	20720, kbA	1
Hepart AG	Buckwheat herb, cut	B120509	2
Hepart AG	Caraway fruit	B-224, kbA	1
Hepart AG	Daisy flower	A130307	1
Hepart AG	Dill fruit	L30057kbA	1
Hepart AG	Equisetum stem, cut	B-695, kbA	1
Hepart AG	Hawthorn flower	13010401	1
Hepart AG	Lavender flower	A130214	4
Hepart AG	Matricaria flower	B-477, kbA	1
Hepart AG	Mullein flower, cut	12170904	2
Hepart AG	Nettle leaf, cut	P234605kbA	1
Hepart AG	Peppermint leaf, cut	B-185	5
Hepart AG	Restharrow root, cut	B130404	3
Hepart AG	Ribwort plantain, cut	20832	5

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Supplier	Substance	Batch	Spectra
Hepart AG	Savory, rubbed	12177205	3
Hepart AG	St. John's wort, cut	B-445,kbA	1
Hepart AG	Stemless carline root	B120726	1
Hepart AG	Thyme, rubbed	A130109	2
Hepart AG	Walnut leaf, cut	A120123	1
Hepart AG	Willowherb, small flo. . .	10326110	2
Herbasinica	Agrimony, cut	11374007	1
Herbasinica	Lavender flower	1488A130830	1
HiperScan	Peppermint leaf, cut		1
Hof-Apotheke,St.Afra	Comfrey root	125041	1
Hubertus Apotheke	Equisetum stem, cut	3831C140403	1
Ichthyol/Phoenix	Fenugreek, powdered	14377205	1
ICHTHYOL-GESELLSCHAFT	Sodium monohydrogenph. . .	Caelo	1
Ichthyol/Phönix	Alchemilla, cut	13141107	3
Ichthyol/Phönix	Zinc orotate dihydrate	12B02-N02	1
Jenne	Aniseed	2700A131015	2
Jenne	Methadone hydrochloride	15B24-B02	1
Jenne	Sodium monohydrogenph. . .	12109003	3
JENNE	Tragacanth, powdered	16110801	1
k	Matricaria flower	1290A140513	1
KBA Ware	Equisetum stem, cut	21879	6
Kenk / Phoenix	Artichoke leaf, cut	1981B130111	3
Kenk / Phoenix	Bitter fennel	2860A130226	5
Kenk / Phoenix	Daisy flower	1210A130307	4
Kenk / Phoenix	European golden rod, . . .	1781B110826	1
Kenk / Phoenix	Fumitory, cut	3881B111013	2
Kenk / Phoenix	Hawthorn leaf with fl. . .	1971A130307	5
Kenk / Phoenix	Lapacho wood, cut	5161A110204	1
Kenk / Phoenix	Raspberry leaf, cut	22781C120508	1
Kenk / Phoenix	Sage leaf, cut	2301A130904	1
Kenk / Phoenix	Turmeric, javanese, cut	6731B130117	1
Kle	Dill fruit	2680A110204	1
Klenk	Abrotani herb, cut	21081301	1
Klenk	Abrotani herb, cut	26011403	1
Klenk	Acorus root, natural, . . .	B130807	1
Klenk	Acorus root, peeled	6701B130870	1
Klenk	Acorus root, peeled	6711B110606	1
Klenk	Acorus root, peeled	6701B120427	7
Klenk	Acorus root, peeled	4797362	1
Klenk	Acorus root, peeled	106212173	1
Klenk	Acorus root, peeled	6701B150407	1
Klenk	Acorus root, peeled	6701B120301	3
Klenk	Acorus root, peeled	6701b130103	1
Klenk	Acorus root, peeled	6701B120817	5
Klenk	Acorus root, peeled	6701b120301	1
Klenk	Agnus castus fruit	7110N090701	1
Klenk	Agnus castus fruit	7110N150121	1
Klenk	Agnus castus fruit	7110A110614	2
Klenk	Agnus castus fruit	12274007	3
Klenk	Agnus castus fruit	7110A130613	1
Klenk	Agnus castus fruit	A130613	1
Klenk	Agnus castus fruit	A110614	3
Klenk	Agnus castus fruit	A120803	1
Klenk	Agrimony, cut	3481C120508	1
Klenk	Alchemilla, cut	3501C121105	2
Klenk	Alchemilla, cut	3501A110301	3
Klenk	Alchemilla, cut	3501B100428	1
Klenk	Alchemilla, cut	3501B090417	1
Klenk	Almonds, bitter, whole	40A0130909	1
Klenk	Almonds, bitter, whole	40A111004	1

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Supplier	Substance	Batch	Spectra
Klenk	Almonds, bitter, whole	40A120924	4
Klenk	Almonds, bitter, whole	40A111117	7
Klenk	Almonds, bitter, whole	40A161206	3
Klenk	Almonds, bitter, whole	40A0161005	1
Klenk	Almonds, bitter, whole	40A130909	9
Klenk	Almonds, bitter, whole	40A150905	1
Klenk	Almonds, bitter, whole	40A161028	4
Klenk	Almonds, bitter, whole	40A161005	1
Klenk	Almonds, bitter, whole	40A150904	8
Klenk	Almonds, bitter, whole	40A-150904	2
Klenk	Almonds, bitter, whole	40A140908	18
Klenk	Almonds, bitter, whole	40A121010	11
Klenk	Angelica root		1
Klenk	Angelica root	6091B130109	1
Klenk	Angelica root	B130109	2
Klenk	Angelica root	6081B170601	1
Klenk	Angelica root	6085B120614	1
Klenk	Angelica root	6081n120110	1
Klenk	Angelica root	6081N120110	13
Klenk	Angelica root	6081B130410	3
Klenk	Angelica root	6081B150701	3
Klenk	Angelica root	6081B130726	1
Klenk	Angelica root	6081b130109	2
Klenk	Angelica root	6081B130109	1
Klenk	Angelica root	6082b130410	1
Klenk	Angelica root	6081B140918	1
Klenk	Aniseed	3113Q01530	1
Klenk	Aniseed	2700A120320	8
Klenk	Aniseed	212M-01530	1
Klenk	Aniseed	2700A150601	5
Klenk	Aniseed	2700A130527	14
Klenk	Aniseed	2700A160511	4
Klenk	Aniseed	2700A140129	6
Klenk	Aniseed	2103311530	1
Klenk	Aniseed	2700A110701	7
Klenk	Aniseed	2700A-110701	1
Klenk	Aniseed	2901311530	1
Klenk	Aniseed	814Q01530	1
Klenk	Aniseed	2700a120320	1
Klenk	Aniseed	2700A121107	1
Klenk	Aniseed	2700A12107	1
Klenk	Aniseed, pounded	2706B100120	1
Klenk	Aniseed, powdered	2704B110824	1
Klenk	Apple, cut	A120302	3
Klenk	Arnica flower	1181B130605	1
Klenk	Artichoke leaf, cut	B121025	2
Klenk	Artichoke leaf, cut	1981B120413	1
Klenk	Artichoke leaf, cut	1981B121025	2
Klenk	Ash leaf, cut	5111A-01491	1
Klenk	Asparagus root, cut	6151B100332	1
Klenk	Asplenium scolopendri. . .	4451B091116	1
Klenk	Asplenium scolopendri. . .	4451B120605	1
Klenk	Barberry root bark, cut	551B120320	1
Klenk	Barberry root bark, cut	551B110128	4
Klenk	Basil, rubbed	3632A110201	3
Klenk	Basil, rubbed	3632a120502	1
Klenk	Basil, rubbed	A120502	1
Klenk	Basil, rubbed	A110201	1
Klenk	Basil, rubbed	3632A120502	4
Klenk	Bean shells, cut	671A-110420	1

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Supplier	Substance	Batch	Spectra
Klenk	Bean shells, cut	671A110301	1
Klenk	Bean shells, cut	C121105	2
Klenk	Bean shells, cut	671C121105	7
Klenk	Bean shells, cut	C120321	2
Klenk	Bean shells, cut	171A110301	1
Klenk	Bean shells, cut	671A110420	9
Klenk	Bean shells, cut	671A100816	2
Klenk	Bean shells, cut	C130620	1
Klenk	Bean shells, cut	671C130620	6
Klenk	Bean shells, cut	671C120321	16
Klenk	Bearberry leaf, cut	2391B120314	6
Klenk	Bearberry leaf, cut	2391b120314	2
Klenk	Bearberry leaf, cut	2391B120719	13
Klenk	Bearberry leaf, cut	2391B07030901	1
Klenk	Bearberry leaf, cut	2391B130328	9
Klenk	Bilberry fruit, dried	2910n130131	1
Klenk	Bilberry fruit, dried	2910N130131	10
Klenk	Bilberry fruit, dried	910N130131	1
Klenk	Bilberry fruit, dried	2910A090717	1
Klenk	Bilberry fruit, dried	2010N110304	1
Klenk	Bilberry fruit, dried	N130131	2
Klenk	Bilberry fruit, dried	2910n110304	1
Klenk	Bilberry fruit, dried	N121022	1
Klenk	Bilberry fruit, dried	2910N121022	7
Klenk	Bilberry fruit, dried	2910N110304	5
Klenk	Bilberry leaf, cut	2191N110516	5
Klenk	Bilberry leaf, cut	4042013	1
Klenk	Bilberry leaf, cut	N110516	1
Klenk	Birch leaf, cut	21061303	1
Klenk	Birch leaf, cut	C120802	1
Klenk	Birch leaf, cut	4021409	1
Klenk	Birch leaf, cut	1901A130218	4
Klenk	Birch leaf, cut	A121130	2
Klenk	Birch leaf, cut	1901A-110726	3
Klenk	Birch leaf, cut	1901C120802	19
Klenk	Birch leaf, cut	F-040413-1	1
Klenk	Birch leaf, cut	1901A121130	23
Klenk	Birch leaf, cut	1901C120508	18
Klenk	Birch leaf, cut	1901A110726	24
Klenk	Birch leaf, cut	1901c120802	1
Klenk	Birch leaf, cut	1901c120508	1
Klenk	Birch leaf, cut	20111201	1
Klenk	Birch leaf, cut	1901A05051801	1
Klenk	Birch leaf, cut	27121301	1
Klenk	Birch leaf, cut	4113A-01481	1
Klenk	Birch leaf, cut	4213I01481	1
Klenk	Birch leaf, cut	1901A140214	1
Klenk	Birch leaf, cut	28101306	1
Klenk	Birch leaf, cut	1901A130318	2
Klenk	Bitter fennel	2866B130206	1
Klenk	Bitter fennel	2866B110318	1
Klenk	Bitter fennel	2880N120418	4
Klenk	Bitter fennel	2880A100503	2
Klenk	Bitter fennel	2860A130513	2
Klenk	Bitter fennel	2860a120412	3
Klenk	Bitter fennel	2860A140224	1
Klenk	Bitter fennel	2860A150617	4
Klenk	Bitter fennel	2860A140224	1
Klenk	Bitter fennel	2860A140612	11
Klenk	Bitter fennel	2860 ,A150617	1

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Supplier	Substance	Batch	Spectra
Klenk	Bitter fennel	2860A140613	2
Klenk	Bitter fennel	2860A110704	4
Klenk	Bitter fennel	28060A140612	1
Klenk	Bitter fennel	3812A-01545	1
Klenk	Bitter fennel	2860A150320	11
Klenk	Bitter fennel	2866B100211	1
Klenk	Bitter orange flower ...	1201B110809	1
Klenk	Bitter orange flower ...	3613m-01445	1
Klenk	Bitter orange flower ...	1201B120822	1
Klenk	Bitter orange peel, cut	511B120830	4
Klenk	Bitter orange peel, cut	2711B111207	1
Klenk	Bitter orange peel, cut	511C130226	1
Klenk	Bitter orange peel, cut	3613M-01531	1
Klenk	Bitter orange peel, cut	B120830	1
Klenk	Bitter orange peel, cut	C130226	3
Klenk	Bitter orange peel, cut	511B110321	2
Klenk	Black cohosh, cut	6721b130528	1
Klenk	Black cohosh, cut	3794377	1
Klenk	Black cohosh, cut	6721B1130528	1
Klenk	Black cohosh, cut	6721B130528	3
Klenk	Black cohosh, cut	6721B130214	10
Klenk	Black cohosh, cut	6721B081208	1
Klenk	Black cohosh, cut	B130528	2
Klenk	Black cumin seed	7330A120703	1
Klenk	Black cumin seed	A120703	1
Klenk	Black mustard seed	7430A120813	2
Klenk	Black mustard seed, p...	A130422	1
Klenk	Black mustard seed, p...	7434A120712	1
Klenk	Black mustard seed, p...	7434A140923	2
Klenk	Black mustard seed, p...	7434A150608	4
Klenk	Black mustard seed, p...	7434a150608	1
Klenk	Black mustard seed, p...	7434A130422	3
Klenk	Black pepper	A130415	2
Klenk	Blackberry leaf, cut	2271B111216	1
Klenk	Blackcurrant leaf, cut	2251a110204	1
Klenk	Blackcurrants	A121106	1
Klenk	Blackcurrants	2990A110620	1
Klenk	Blackthorn flower	2612E-01468	1
Klenk	Blackthorn flower, ru...	N101109	2
Klenk	Blackthorn flower, ru...	1150n101109	1
Klenk	Blessed thistle, cut	A110517	1
Klenk	Blue bottle flower wi...		1
Klenk	Boldo leaf, cut	1911A100714	6
Klenk	Boldo leaf, cut	1911B090709	1
Klenk	Buckwheat herb, cut	4581B120509	3
Klenk	Burdock root, cut	6161A101206	1
Klenk	Burdock root, cut	6161A-101206	1
Klenk	Burdock root, cut	A120206	1
Klenk	Burdock root, cut	6161A120208	3
Klenk	Burdock root, cut	6161A080709	1
Klenk	Burdock root, cut	6161A-120103	1
Klenk	Burdock root, cut	6161A120103	1
Klenk	Burdock root, cut	A130214	1
Klenk	Calendula flower	C120321	1
Klenk	Calendula flower	1250A110511	1
Klenk	Calendula flower	1241B130517	1
Klenk	Calendula flower	1241B120312	1
Klenk	Calendula flower, cut	1241N151209	1
Klenk	Calendula flower, cut	1241B110118	2
Klenk	Calendula flower, cut	1241B120419	2

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Supplier	Substance	Batch	Spectra
Klenk	Calendula flower, cut	112211448	1
Klenk	Calendula flower, cut	1241B130927	1
Klenk	Calendula flower, cut	1240A110418	1
Klenk	Calendula flower, cut	204311448	1
Klenk	Calendula flower, cut	1241B130321	5
Klenk	Calendula flower, cut	3013E1448	1
Klenk	Calendula flower, cut	1241B150902	1
Klenk	Calendula flower, cut	B130517	2
Klenk	Calendula flower, cut	1241B130517	5
Klenk	Calendula flower, cut	1241C120321	4
Klenk	Calendula flower, cut	1241B160530	1
Klenk	Calendula flower, cut	1241B140211	1
Klenk	Caraway fruit	2770A110601	9
Klenk	Caraway fruit	A120905	3
Klenk	Caraway fruit	2770a120905	2
Klenk	Caraway fruit	2770A130521	12
Klenk	Caraway fruit	2770A140708	3
Klenk	Caraway fruit	1810A-01537	1
Klenk	Caraway fruit	2770A120403	14
Klenk	Caraway fruit	2770A131008	2
Klenk	Caraway fruit	2770A130910	1
Klenk	Caraway fruit	412091-1-P	1
Klenk	Caraway fruit	2770A110818	8
Klenk	Caraway fruit	5213A1537	1
Klenk	Caraway fruit	2270A130521	1
Klenk	Cardamom fruit	A110810	3
Klenk	Cardamom fruit	2750A110810	2
Klenk	Cardamom fruit	A130807	1
Klenk	Centaury, cut	3711B111216	1
Klenk	Centaury, cut	3711B-111216	1
Klenk	Centaury, cut	B120628	1
Klenk	Ceylon cinnamon, fine...	614a120411	1
Klenk	Ceylon cinnamon, fine...	614b121024	1
Klenk	Ceylon cinnamon, fine...	614B120411	2
Klenk	Ceylon cinnamon, fine...	611B100628	1
Klenk	Ceylon cinnamon, fine...	615B130325	3
Klenk	Ceylon cinnamon, fine...	614B121010	2
Klenk	Ceylon cinnamon, fine...	614B121024	4
Klenk	Chelidonium majus her...	3731B100205	1
Klenk	Chelidonium majus her...	3731A110301	6
Klenk	Chelidonium majus her...	3731A130904	2
Klenk	Chelidonium majus her...	1406111632	1
Klenk	Chelidonium majus her...	3731A120611	4
Klenk	Chelidonium majus her...	4711E-01632	1
Klenk	Chelidonium majus her...	3731K120904	4
Klenk	Chickweed, cut	4551B090528	1
Klenk	Chickweed, cut	4551b110222	1
Klenk	Chicory herb, cut	3751A080902	1
Klenk	Chicory herb, cut	4510I-01634	1
Klenk	Chicory herb, cut	3751A120307	6
Klenk	Chicory herb, cut	A120123	2
Klenk	Chicory herb, cut	3751A120123	2
Klenk	Chicory herb, cut	3751a120307	1
Klenk	Chicory herb, cut	3751A-100118	1
Klenk	Chicory herb, cut	3751c120614	1
Klenk	Chicory root, cut	66221A101202	1
Klenk	Chicory root, cut	6221A130304	1
Klenk	Chicory root, cut	A130304	1
Klenk	Chicory root, cut	6221A090311	1
Klenk	Cinchona bark, cut	601B130415	1

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Supplier	Substance	Batch	Spectra
Klenk	Cinchona bark, cut	601B130415	1
Klenk	Cinnamon rods (Ceylon...	A101018	1
Klenk	Cinnamon rods (Ceylon...	B121016	1
Klenk	Cinnamon rods (Ceylon...	610A101018	1
Klenk	Cinnamon, cut	610A130927	1
Klenk	Cinnamon, cut	610A101018	1
Klenk	Clove	1260A130903	3
Klenk	Clove	1260A101223	1
Klenk	Clove	1260A110608	5
Klenk	Clove	A120328	1
Klenk	Clove	1260A120328	5
Klenk	Clove	1260A100617	2
Klenk	Clove	1260A150304	2
Klenk	Coltsfoot leaf, cut	2021B120601	5
Klenk	Coltsfoot leaf, cut	KS100061	1
Klenk	Coltsfoot leaf, cut	5011301	1
Klenk	Coltsfoot leaf, cut	20021301	1
Klenk	Coltsfoot leaf, cut	2021B121203	5
Klenk	Coltsfoot leaf, cut	2021b121204	1
Klenk	Coltsfoot leaf, cut	B120124	1
Klenk	Coltsfoot leaf, cut	2021B130227	11
Klenk	Coltsfoot leaf, cut	2020B120124	1
Klenk	Coltsfoot leaf, cut	2021B140131	1
Klenk	Coltsfoot leaf, cut	B130227	1
Klenk	Coltsfoot leaf, cut	23121302	1
Klenk	Coltsfoot leaf, cut	5122013a	1
Klenk	Coltsfoot leaf, cut	2021B150407	1
Klenk	Coltsfoot leaf, cut	2021B111005	1
Klenk	Coltsfoot leaf, cut	8061207	1
Klenk	Coltsfoot leaf, cut	2021C140730	1
Klenk	Coltsfoot leaf, cut	14111302	1
Klenk	Coltsfoot leaf, cut	2021B120124	4
Klenk	Coltsfoot leaf, cut	2021C130326	8
Klenk	Coltsfoot leaf, cut	26091301	1
Klenk	Coltsfoot leaf, cut	11101202	1
Klenk	Comfrey herb, cut	4561B100518	2
Klenk	Comfrey root	6241b130619	1
Klenk	Comfrey root	6241B130724	7
Klenk	Comfrey root	6244B130624	1
Klenk	Comfrey root	6241b130724	1
Klenk	Comfrey root	6241B131009	1
Klenk	Comfrey root	6241b120807	1
Klenk	Comfrey root	6241B100715	1
Klenk	Comfrey root	6241B120531	3
Klenk	Comfrey root	6241B120807	3
Klenk	Comfrey root	6241B121214	2
Klenk	Comfrey root	B130619	1
Klenk	Comfrey root	6241B130619	8
Klenk	Comfrey root	6241B130312	3
Klenk	Comfrey root	6241B06110202	1
Klenk	Common wormwood herb,...	3591A11119	1
Klenk	Common wormwood herb,...	3591A120123	7
Klenk	Common wormwood herb,...	2591A130218	1
Klenk	Common wormwood herb,...	3591a130218	2
Klenk	Common wormwood herb,...	3591A130218	9
Klenk	Common wormwood herb,...	A120123	2
Klenk	Common wormwood herb,...	3591a120123	1
Klenk	Coriander	2709A130129	1
Klenk	Coriander	2790A151117	1
Klenk	Coriander	2790A130129	2

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Supplier	Substance	Batch	Spectra
Klenk	Coriander	2790A161111	5
Klenk	Coriander	2790a121023	1
Klenk	Coriander	2790A121023	7
Klenk	Coriander	A121023	3
Klenk	Cottonwood bud	3260A120828	1
Klenk	Cowberry leaf, cut	2431B101006	2
Klenk	Daisy flower	1210A120215	3
Klenk	Daisy flower	1210a071301	1
Klenk	Daisy flower	A130705	1
Klenk	Daisy flower	1210A110223	1
Klenk	Damiana leaf, cut	12064101	1
Klenk	Damiana leaf, cut	1990A130206	1
Klenk	Damiana leaf, cut	A130206	2
Klenk	Dandelion herb with r...	6611B110929	2
Klenk	Dandelion herb with r...	6611B110131	1
Klenk	Dandelion herb with r...	6611B130314	2
Klenk	Dandelion herb with r...	6611B-120620	1
Klenk	Dandelion herb with r...	6611B120620	19
Klenk	Dandelion herb with r...	6611B160613	1
Klenk	Dandelion herb with r...	6611B1104104	1
Klenk	Dandelion herb with r...	5122013b	1
Klenk	Dandelion herb with r...	6611B110104	5
Klenk	Dandelion herb with r...	6611B-131206	1
Klenk	Dandelion herb with r...	6611B090306	1
Klenk	Dandelion herb with r...	6611A110104	1
Klenk	Dandelion root, cut	A120606	1
Klenk	Dandelion root, cut	6621A140114	3
Klenk	Dandelion root, cut	6621N130813	6
Klenk	Dandelion root, cut	6621A140114	3
Klenk	Dandelion root, cut	N130813	1
Klenk	Dandelion root, cut	6621A141027	5
Klenk	Dandelion root, cut	6621A160111	1
Klenk	Dandelion root, cut	6101202	1
Klenk	Dandelion root, cut	6621A120208	6
Klenk	Dandelion root, cut	6621A110420	1
Klenk	Dandelion root, cut	6621A120606	15
Klenk	Devil's claw root	6331B120508	3
Klenk	Devil's claw root	6331B130129	5
Klenk	Devil's claw root	10111204	1
Klenk	Dill fruit	2680a120312	1
Klenk	Dill fruit	2680A-120312	1
Klenk	Dill fruit	A120312	1
Klenk	Dill fruit	2680A120312	7
Klenk	Dill fruit	2680A121211	3
Klenk	Dill herb, cut	3531B110726	1
Klenk	Elder berries	3010N120921	3
Klenk	Elder flower, rubbed	1571A-110223	1
Klenk	Elder flower, rubbed	1571A141126	1
Klenk	Elder flower, rubbed	1571A130627	2
Klenk	Elder flower, rubbed	26061201	1
Klenk	Elder flower, rubbed	21091201	1
Klenk	Elder flower, rubbed	1571A110125	2
Klenk	Elder flower, rubbed	16061201	1
Klenk	Elder flower, rubbed	1571A130930	3
Klenk	Elder flower, rubbed	1571A110223	16
Klenk	Elder flower, rubbed	A120215	1
Klenk	Elder flower, rubbed	13021301	1
Klenk	Elder flower, rubbed	1571a120215	1
Klenk	Elder flower, rubbed	1571a1211	1
Klenk	Elder flower, rubbed	A121121	1

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Supplier	Substance	Batch	Spectra
Klenk	Elder flower, rubbed	1571A1202015	1
Klenk	Elder flower, rubbed	1571A120215	4
Klenk	Elder flower, rubbed	1571A121121	19
Klenk	Elder root, cut	6281B110427	4
Klenk	Elecampane rhizome, cut	6341B100426	2
Klenk	Elecampane rhizome, cut	6311141B130423	1
Klenk	Elecampane rhizome, cut	6341B130423	3
Klenk	Elecampane rhizome, cut	B130423	3
Klenk	Elecampane rhizome, cut	6341B120611	2
Klenk	Eleutherococcus, cut	7011A101206	1
Klenk	Eleutherococcus, cut	7011A110714	1
Klenk	Eleutherococcus, cut	7011A121204	1
Klenk	Elm bark, cut	841a120413	1
Klenk	Elm bark, cut	841A1101120	1
Klenk	Equisetum stem, cut	3831A120903	7
Klenk	Equisetum stem, cut	3831A111124	4
Klenk	Equisetum stem, cut	3831A120018	1
Klenk	Equisetum stem, cut	3831A120529	8
Klenk	Equisetum stem, cut	3831a120611	1
Klenk	Equisetum stem, cut	3831A110922	1
Klenk	Equisetum stem, cut	3831A1230726	1
Klenk	Equisetum stem, cut	3831A110601	1
Klenk	Equisetum stem, cut	4713U01642	1
Klenk	Equisetum stem, cut	3831A111124	1
Klenk	Equisetum stem, cut	3831A120611	10
Klenk	Equisetum stem, cut	2213U01642	1
Klenk	Equisetum stem, cut	3831C131104	1
Klenk	Equisetum stem, cut	3831A120726	18
Klenk	Equisetum stem, cut	3831c131104	1
Klenk	Equisetum stem, cut	3831A121018	6
Klenk	Equisetum stem, cut	4413Q1642	1
Klenk	Eucalyptus leaf, cut	B120419	1
Klenk	Eucalyptus leaf, cut	2011B130306	4
Klenk	Eucalyptus leaf, cut	2011b130306	1
Klenk	Eucalyptus leaf, cut	B130306	2
Klenk	Eucalyptus leaf, cut	2011B130306-35294110	1
Klenk	Eucalyptus leaf, cut	2011B120419	5
Klenk	Euphrasy herb, cut	3871B130430	1
Klenk	Euphrasy herb, cut	B130430	1
Klenk	Euphrasy herb, cut	B101206	1
Klenk	Euphrasy herb, cut	15029806	1
Klenk	European golden rod, ...	1781B110706	1
Klenk	Fenugreek	7260A130603	3
Klenk	Fenugreek	A130603	1
Klenk	Fenugreek	9011301	1
Klenk	Fenugreek	8061301	1
Klenk	Fenugreek	7260A120118	2
Klenk	Fenugreek	7260A110530	2
Klenk	Fenugreek	A120118	2
Klenk	Fenugreek, powdered	A110201	1
Klenk	Fenugreek, powdered	7264A110201	9
Klenk	Fenugreek, powdered	12082014A	1
Klenk	Flax weed herb, cut	4011B131115	3
Klenk	Flax weed herb, cut	4011B121207	2
Klenk	Frangula bark, cut	661B-110412	1
Klenk	Frangula bark, cut	661B130306	1
Klenk	Frangula bark, cut	661B110412	4
Klenk	Frangula bark, cut	661B-090903	1
Klenk	Frangula bark, cut	6621B110412	1
Klenk	Fraxinella root, cut	6271B140708	1

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Supplier	Substance	Batch	Spectra
Klenk	Fumitory, cut	B120410	1
Klenk	Fumitory, cut	3881B100127	1
Klenk	Galeopsis herb, cut	3911a130320	1
Klenk	Galeopsis herb, cut	3911A080409	1
Klenk	Galeopsis herb, cut	3911A130110	3
Klenk	Galeopsis herb, cut	3911A090219	2
Klenk	Gentian root, cut	6311a120723	2
Klenk	Gentian root, cut	6311B140704	1
Klenk	Gentian root, cut	1911E-02142	1
Klenk	Gentian root, cut	6311A120723	3
Klenk	Gentian root, cut	6311B130205	2
Klenk	Ginger, peeled	6951B110822	1
Klenk	Ginger, peeled	6951B110119	1
Klenk	Ginger, peeled	6951B100302	1
Klenk	Ginger, peeled	6951B130110	1
Klenk	Ginger, peeled, powde...	6954B121030	2
Klenk	Ginger, peeled, powde...	6954B170127	1
Klenk	Ginger, peeled, powde...	6954B160429	5
Klenk	Ginger, peeled, powde...	6954B16029	1
Klenk	Ginger, peeled, powde...	6954B130418	2
Klenk	Ginger, peeled, powde...	6954B160929	2
Klenk	Ginger, peeled, powde...	B121030	2
Klenk	Ginger, peeled, powde...	6954B110801	1
Klenk	Ginger, peeled, powde...	KS200260	1
Klenk	Goat's rue, cut	3901B140801	1
Klenk	Goat's rue, cut	3901C110905	1
Klenk	Ground ivy herb, cut	3991B110304	1
Klenk	Ground ivy herb, cut	3991B130502	2
Klenk	Hamamelis leaf, cut	B110214	1
Klenk	Hamamelis leaf, cut	2051B110214	1
Klenk	Hawthorn flower	1351B111207	4
Klenk	Hawthorn flower	B1112107	1
Klenk	Hawthorn fruit	2806B110818	2
Klenk	Hawthorn fruit	2806B121203	2
Klenk	Hawthorn leaf with fl...	1971a120813	2
Klenk	Hawthorn leaf with fl...	1971A120215	3
Klenk	Hawthorn leaf with fl...	1971A110620	5
Klenk	Hawthorn leaf with fl...	1971a120215	1
Klenk	Hawthorn leaf with fl...	1971A120813	17
Klenk	Hawthorn leaf with fl...	A130307	1
Klenk	Hawthorn leaf with fl...	1971A130307-35014110	1
Klenk	Hawthorn leaf with fl...	28101307	1
Klenk	Hawthorn leaf with fl...	1972A120727	1
Klenk	Hawthorn leaf with fl...	1971A120813-34103101	1
Klenk	Hawthorn leaf with fl...	1971A130307-3447	1
Klenk	Hawthorn leaf with fl...	1971A120727	12
Klenk	Hawthorn leaf with fl...	14101301	1
Klenk	Hawthorn leaf with fl...	20121302	1
Klenk	Hay flower	10192103	1
Klenk	Hay flower	A130304	1
Klenk	Hay flower	1400A120116	1
Klenk	Heather flower, rubbed	13014202	1
Klenk	Henna powder	20747A111004	1
Klenk	Henna powder	2074A111004	1
Klenk	Hop strobile	1451b130409	1
Klenk	Hop strobile	1451B140408	1
Klenk	Hop strobile	1451B130409	1
Klenk	Hop strobile	B130409	1
Klenk	Hop strobile	1451B130409	7
Klenk	Hop strobile	1451b130107	1

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Supplier	Substance	Batch	Spectra
Klenk	Hop strobile	1450A110712	1
Klenk	Hop strobile	1451B120202	6
Klenk	Hop strobile	1451B111004	1
Klenk	Hop strobile	1451B120817	7
Klenk	Hop strobile	20071301	1
Klenk	Hop strobile	1451B-120817	1
Klenk	Horse chestnut flower...	1440A110311	3
Klenk	Horse chestnut leaf, ...	255100903	1
Klenk	Horse chestnut leaf, ...	N130124	2
Klenk	Horse chestnut leaf, ...	2551B081223	1
Klenk	Horse chestnut leaf, ...	2551N130124	3
Klenk	Iceland moss, cut	5191A140828	1
Klenk	Iceland moss, cut	5191N110609	1
Klenk	Ispaghula seed	20071302	1
Klenk	Ispaghula seed	7560A140203	1
Klenk	Ispaghula seed	7560A130710	1
Klenk	Ispaghula seed	7560A150420	3
Klenk	Ispaghula seed	7560A130418	2
Klenk	Ispaghula seed	7560A160229	1
Klenk	Ispaghula seed	7560A120828	7
Klenk	Ivy leaf, cut	B130118	1
Klenk	Jasmine flower	1460A110505	1
Klenk	Java tea, cut	2221B12112	1
Klenk	Java tea, cut	2221B110718	6
Klenk	Java tea, cut	B110718	1
Klenk	Java tea, cut	B121112	3
Klenk	Java tea, cut	17121304	1
Klenk	Juniper	2890a120709	1
Klenk	Juniper	A120709	3
Klenk	Juniper	2890A101201	5
Klenk	Juniper	2890A120709	12
Klenk	Juniper	2890A130513	2
Klenk	Juniper, pounded	2896B121016	7
Klenk	Kaolin, heavy	424A100819	2
Klenk	Kaolin, heavy	424A130507	2
Klenk	Kaolin, heavy	45131I01190	1
Klenk	Kelp, cut	1051A110920	1
Klenk	Knotgrass, cut	4301A121120	3
Klenk	Knotgrass, cut	4301A120912	1
Klenk	Ladys bedstraw herb,...	3921C130226	1
Klenk	Ladys bedstraw herb,...	3921B12030	1
Klenk	Lapacho wood, cut	13298302	1
Klenk	Large waybread herb, ...	4281N110404	1
Klenk	Large waybread herb, ...	4281N111121	5
Klenk	Large waybread herb, ...	N111121	1
Klenk	Laurel leaf	B110809	1
Klenk	Laurel leaf, cut	B110809	2
Klenk	Lavender flower	1489A1203	1
Klenk	Lavender flower	1488B130604	4
Klenk	Lavender flower	313U-01462	1
Klenk	Lavender flower	1489A100125	1
Klenk	Lavender flower	1489A130214	16
Klenk	Lavender flower	1489A120103	19
Klenk	Lavender flower	1488A111201	2
Klenk	Lavender flower	1488A120803	3
Klenk	Lavender flower	1488B130111	2
Klenk	Lemon grass, cut	7721A120906	1
Klenk	Lemon grass, cut	A130907	1
Klenk	Lemon grass, cut	7721A130708	1
Klenk	Lemon grass, cut	A120906	1

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Supplier	Substance	Batch	Spectra
Klenk	Lemon peel, cut	621A091016	1
Klenk	Lemon peel, cut	621A130221	1
Klenk	Lemon peel, cut	A130221	3
Klenk	Lemon peel, cut	B130521	1
Klenk	Lemon verbena leaf, cut	2411B110408	2
Klenk	Lime flower, cut	1611B131220	1
Klenk	Lime flower, cut	1611B1010004	1
Klenk	Lime flower, cut	1611B130307	3
Klenk	Lime flower, cut	B130307	2
Klenk	Lime flower, cut	Pr.Nr.4411A-01474	1
Klenk	Lime flower, cut	B130905	4
Klenk	Lime flower, cut	1611A121120	7
Klenk	Lime flower, cut	1611B130905	5
Klenk	Lime flower, cut	1611B110421	2
Klenk	Lime flower, cut	1611B121105	4
Klenk	Lime flower, cut	1611B120827	11
Klenk	Lime flower, cut	1611B111011	5
Klenk	Lime flower, cut	1611a121120	2
Klenk	Lime leaf, cut	2471B120502	1
Klenk	Linseed	7307A131021	1
Klenk	Linseed	7307A-130722	1
Klenk	Linseed	7307A131104	8
Klenk	Linseed	2002285	1
Klenk	Linseed	3707A140526	1
Klenk	Linseed	7307A140526	3
Klenk	Linseed	7300A111107	3
Klenk	Linseed	7500A140556	1
Klenk	Linseed	7300A141201	4
Klenk	Linseed	7307a131104	1
Klenk	Linseed	1910212240	1
Klenk	Linseed	7308A150710	2
Klenk	Linseed	7308A111107	3
Klenk	Linseed	7307A121212	1
Klenk	Linseed	903312240	1
Klenk	Linseed	7300A130110	7
Klenk	Linseed	7307A130110	15
Klenk	Linseed	7307A150710	3
Klenk	Linseed	7307A130124	1
Klenk	Linseed	1913Q-02240	1
Klenk	Linseed	7307A-130110	1
Klenk	Linseed	A130110	1
Klenk	Linseed	7308A130110	4
Klenk	Linseed	7307A130722	5
Klenk	Linseed	7307a111107	1
Klenk	Linseed	7308A150414	1
Klenk	Linseed	7300A130722	8
Klenk	Linseed	7307A160414	1
Klenk	Linseed	7300A170306	2
Klenk	Liquorice root, peeled	6381A121126	27
Klenk	Liquorice root, peeled	6381A130425	1
Klenk	Liquorice root, peeled	A130426	1
Klenk	Liquorice root, peeled	6381a121126	1
Klenk	Liquorice root, peeled	6381A130426	19
Klenk	Liquorice root, peeled	6381A110531	2
Klenk	Liquorice root, peeled	6381A140109	2
Klenk	Liquorice root, peeled	6381a111004	1
Klenk	Liquorice root, peeled	6381A130820	4
Klenk	Liquorice root, peeled	A130820	3
Klenk	Liquorice root, peeled	638A130820	1
Klenk	Liquorice root, peeled	6381A120806	3

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Supplier	Substance	Batch	Spectra
Klenk	Liquorice root, natur...	6390A101020	1
Klenk	Liquorice root, natur...	6391A110421	4
Klenk	Liquorice root, natur...	6391A080905	4
Klenk	Lovage root, cut	6371B121029	3
Klenk	Lovage root, cut	B110228	1
Klenk	Lovage root, cut	6371B-121029	1
Klenk	Lovage root, cut	6371A080508	1
Klenk	Lovage root, cut	B121029	1
Klenk	Lungwort herb, cut	4331B111205	1
Klenk	Lungwort herb, cut	4331A120813	1
Klenk	Lycopodium herb, cut	4111B110428	1
Klenk	Maize style, cut	5581A111206	1
Klenk	Maize style, cut	5581A081204	1
Klenk	Maize style, cut	A110411	1
Klenk	Male speedwell wort, ...	4661C131104	1
Klenk	Male speedwell wort, ...	4661C130226	27
Klenk	Male speedwell wort, ...	4661A090318	1
Klenk	Male speedwell wort, ...	4661C13026	1
Klenk	Male speedwell wort, ...	4661B101011	1
Klenk	Male speedwell wort, ...	4661c130226-34343111	1
Klenk	Male speedwell wort, ...	4661C130226-32743106	1
Klenk	Male speedwell wort, ...	4661C-111011	1
Klenk	Male speedwell wort, ...	4661C120802	13
Klenk	Male speedwell wort, ...	6661C130226	1
Klenk	Male speedwell wort, ...	4661C2004	1
Klenk	Male speedwell wort, ...	4661c120321	1
Klenk	Male speedwell wort, ...	4661C111011	13
Klenk	Male speedwell wort, ...	4661B110916	1
Klenk	Male speedwell wort, ...	4661c120802	1
Klenk	Male speedwell wort, ...	C130226	5
Klenk	Male speedwell wort, ...	4661B110121	2
Klenk	Male speedwell wort, ...	C120321	1
Klenk	Mallow flower, cut	B130829	3
Klenk	Mallow flower, cut	150B111215	1
Klenk	Mallow flower, cut	1501b111215	1
Klenk	Mallow flower, cut	1501B130829	3
Klenk	Mallow flower, cut	1501B100408	1
Klenk	Mallow flower, cut	1910211464	1
Klenk	Mallow flower, cut	1501b110207	1
Klenk	Mallow flower, cut	1501B-120427	1
Klenk	Mallow flower, cut	1501B111215	1
Klenk	Mallow flower, cut	10357908	2
Klenk	Mallow flower, cut	B120427	1
Klenk	Mallow flower, cut	1501B120427	10
Klenk	Mallow leaf, cut	B130225	1
Klenk	Mallow leaf, cut	2131B10529	1
Klenk	Mallow leaf, cut	2131B130225	4
Klenk	Manna, cut	5221A120509	10
Klenk	Manna, cut	5221A150107	1
Klenk	Manna, cut	5221A140210	4
Klenk	Manna, cut	5221A110817	1
Klenk	Marian thistle fruit	7180A120725	1
Klenk	Marian thistle fruit	7180A130219	1
Klenk	Marian thistle fruit	7180A132019	1
Klenk	Marian thistle fruit	A120725	1
Klenk	Marian thistle fruit	7180A090929	1
Klenk	Marian thistle fruit	7180A110209	2
Klenk	Marian thistle herb, ...	2011402	1
Klenk	Marian thistle herb, ...	3701a111207	1
Klenk	Marian thistle herb, ...	3701B130318	5

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Supplier	Substance	Batch	Spectra
Klenk	Marian thistle herb, ...	3701A111207	10
Klenk	Marian thistle herb, ...	3701B120717	3
Klenk	Marian thistle herb, ...	B110728	1
Klenk	Marian thistle herb, ...	3701B111117	1
Klenk	Marian thistle herb, ...	11041310	1
Klenk	Marian thistle herb, ...	3701A100916	2
Klenk	Marian thistle herb, ...	913E-01627	1
Klenk	Marjoram herb, rubbed	4881a101025	1
Klenk	Marjoram herb, rubbed	12345678	1
Klenk	Marjoram herb, rubbed	A101025	2
Klenk	Marjoram herb, rubbed	4881A1311105	1
Klenk	Marjoram herb, rubbed	4881A101025	15
Klenk	Marrubium vulgare her...	13289102	1
Klenk	Marrubium vulgare her...	4141A130110	1
Klenk	Marshmallow root, pee...	6074B100416	1
Klenk	Marshmallow root, pee...	6071A130612	4
Klenk	Marshmallow root, pee...	6071A-120314	1
Klenk	Marshmallow root, pee...	6071a130408	1
Klenk	Marshmallow root, pee...	6071B091207	1
Klenk	Marshmallow root, pee...	A130408	3
Klenk	Marshmallow root, pee...	130116	1
Klenk	Marshmallow root, pee...	6071A120314	10
Klenk	Maté leaf, cut	2141a111213	1
Klenk	Maté leaf, cut	2131A111213	1
Klenk	Maté leaf, cut	2141A111213	16
Klenk	Matricaria flower	1290B130415	35
Klenk	Matricaria flower	1290A120529	1
Klenk	Matricaria flower	2310211452	1
Klenk	Matricaria flower	1290A110825	1
Klenk	Matricaria flower	1290a120620	1
Klenk	Matricaria flower	1290B140123	2
Klenk	Matricaria flower	1290A120404	1
Klenk	Matricaria flower	1290B130415	3
Klenk	Matricaria flower	1290B140624	1
Klenk	Matricaria flower	1290A140508	1
Klenk	Matricaria flower	1290A-120620	1
Klenk	Matricaria flower	1290A150618	1
Klenk	Matricaria flower	1290A120601	2
Klenk	Matricaria flower	1290A20404	1
Klenk	Matricaria flower	4100113002	2
Klenk	Matricaria flower	1290A120529	5
Klenk	Matricaria flower	1290A120601	14
Klenk	Matricaria flower	1290A110421	1
Klenk	Matricaria flower	1290A130502	1
Klenk	Matricaria flower	1290A120620	13
Klenk	Matricaria flower	1290A120404	6
Klenk	Matricaria flower	14111314	1
Klenk	Matricaria flower	1290A110607	1
Klenk	Matricaria flower	11101302	1
Klenk	Matricaria flower	A130502	1
Klenk	Matricaria flower	27111204	1
Klenk	Matricaria flower	1290A120403	3
Klenk	Matricaria flower	1290A12061	1
Klenk	Matricaria flower	A120529	1
Klenk	Matricaria flower	A130516	1
Klenk	Matricaria flower	B130415	2
Klenk	Matricaria flower	1290A130516	3
Klenk	Matricaria flower	1290A130502	1
Klenk	Matricaria flower	16121301	1
Klenk	Matricaria flower	A120529	1

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Supplier	Substance	Batch	Spectra
Klenk	Matricaria flower	1290A130516	9
Klenk	Meadowsweet flower, r...	A120312	1
Klenk	Melilot herb, cut	4151A120912	1
Klenk	Melilot herb, cut	A110324	6
Klenk	Melilot herb, cut	4151A110324	8
Klenk	Melissa leaf, cut	2161A121029	3
Klenk	Melissa leaf, cut	2161A151209	1
Klenk	Melissa leaf, cut	2161A121206	2
Klenk	Melissa leaf, cut	27091201	1
Klenk	Melissa leaf, cut	2161A101216	1
Klenk	Melissa leaf, cut	2161A110818	1
Klenk	Melissa leaf, cut	111207	1
Klenk	Melissa leaf, cut	2161A120718	11
Klenk	Melissa leaf, cut	2161A121009	14
Klenk	Melissa leaf, cut	2807211503	1
Klenk	Melissa leaf, cut	2161A121009/PN:1198	1
Klenk	Melissa leaf, cut	2161A111207	15
Klenk	Mistletoe, cut	4691A120507	2
Klenk	Mistletoe, cut	4691a130307	1
Klenk	Mistletoe, cut	4691A-120507	1
Klenk	Mistletoe, cut	4691A130307	7
Klenk	Mistletoe, cut	1512211695	1
Klenk	Mistletoe, cut	4691A110816	2
Klenk	Mistletoe, cut	4691A120419	6
Klenk	Mistletoe, cut	4691A121122-35454110	1
Klenk	Mistletoe, cut	2901311695	1
Klenk	Mistletoe, cut	4961A120419	1
Klenk	Mistletoe, cut	4691A121122	9
Klenk	Mistletoe, cut	110816	1
Klenk	Mistletoe, cut	4691a121122	1
Klenk	Motherwort herb, cut	4071A-100707	1
Klenk	Mullein flower, cut	1650A100608	1
Klenk	Mullein flower, cut	1651b130820	2
Klenk	Mullein flower, cut	1650A111018	3
Klenk	Mullein flower, cut	1651B121109	20
Klenk	Mullein flower, cut	1651B150722	1
Klenk	Mullein flower, cut	A120612	1
Klenk	Mullein flower, cut	1650A120612	1
Klenk	Mullein flower, cut	1651B120315	3
Klenk	Mullein flower, cut	1651B140324	2
Klenk	Mullein flower, cut	1651B130820	5
Klenk	Mullein flower, cut	1651B110203	2
Klenk	Myrrh	3351A121004	1
Klenk	Myrrh	3351A160330	1
Klenk	Myrrh	3351A120514	1
Klenk	Myrrh	3351A130902	1
Klenk	Nettle leaf, cut	2381A130703	12
Klenk	Nettle leaf, cut	2381A150109	1
Klenk	Nettle leaf, cut	2381A141124	1
Klenk	Nettle leaf, cut	2381A140221	1
Klenk	Nettle leaf, cut	114Q-03054	1
Klenk	Nettle leaf, cut	1107211689	1
Klenk	Nettle leaf, cut	A130122	1
Klenk	Nettle leaf, cut	2381a120619	4
Klenk	Nettle leaf, cut	2381A-121010	1
Klenk	Nettle leaf, cut	2381A110809	1
Klenk	Nettle leaf, cut	A110913	1
Klenk	Nettle leaf, cut	2381A121010	1
Klenk	Nettle leaf, cut	2381A-120619	1
Klenk	Nettle leaf, cut	1913A-03054	1

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Supplier	Substance	Batch	Spectra
Klenk	Nettle leaf, cut	2381a130122	1
Klenk	Nettle leaf, cut	4513E3054	1
Klenk	Nettle leaf, cut	A130703	1
Klenk	Nettle leaf, cut	2381A151012	1
Klenk	Nettle root, cut	9931B120927	1
Klenk	Nettle root, cut	6631N110513	1
Klenk	Nettle seed	7470A110418	1
Klenk	Nettle seed	7470A151009	1
Klenk	Nettle seed	2021505	1
Klenk	Nettle seed	7470A170130	1
Klenk	Nettle seed	7470A160928	2
Klenk	Nutmeg, powdered (spi...	7325A130515	1
Klenk	Nutmeg, powdered (spi...	A130304	2
Klenk	Nutmeg, powdered (spi...	7325A120903	2
Klenk	Nutmeg, powdered (spi...	7325A130304	1
Klenk	Oak bark, cut	C-280513-2	1
Klenk	Oak bark, cut	761A110816	9
Klenk	Oak bark, cut	761A110816	1
Klenk	Oak bark, cut	761A090420	1
Klenk	Oak bark, cut	761A110816	1
Klenk	Olive leaf	2211B130425	3
Klenk	Olive leaf	2211B150818	1
Klenk	Olive leaf	2211B120417	2
Klenk	Olive leaf	2211B131025	1
Klenk	Orange peel, cut	531A091125	3
Klenk	Orange peel, cut	531a130204	1
Klenk	Orange peel, cut	531A130204	5
Klenk	Oregano herb	4221A120315	2
Klenk	Orris root	B111013	1
Klenk	Orris root	B130102	1
Klenk	Orris root	6831B111013	1
Klenk	Parsley root, cut	6441A150811	1
Klenk	Parsley root, cut	6441A120283	1
Klenk	Parsley root, cut	6441A121024	4
Klenk	Parsley root, cut	6441A120606	5
Klenk	Parsley seed	7370A091120	2
Klenk	Parsley seed	7370A09120	1
Klenk	Passionflower herb, cut	4231A120329	2
Klenk	Passionflower herb, cut	A120329	2
Klenk	Passionflower herb, cut	4231A-110913	1
Klenk	Peony root, cut	6421B120327	1
Klenk	Peony root, cut	B110916	2
Klenk	Peppermint leaf, cut	2161A120718	3
Klenk	Peppermint leaf, cut	2183A120913	2
Klenk	Peppermint leaf, cut	2161A121029	16
Klenk	Peppermint leaf, cut	2161A-121206	1
Klenk	Peppermint leaf, cut	2161A121009	6
Klenk	Peppermint leaf, cut	A130806	1
Klenk	Peppermint leaf, cut	4513E1503	1
Klenk	Peppermint leaf, cut	1913A-01505	1
Klenk	Peppermint leaf, cut	4113Q1505	1
Klenk	Peppermint leaf, cut	CH.2161B080818	1
Klenk	Peppermint leaf, cut	2161A130806	7
Klenk	Peppermint leaf, cut	2181A-120913	1
Klenk	Peppermint leaf, cut	2181A13020	1
Klenk	Peppermint leaf, cut	2161A110207	1
Klenk	Peppermint leaf, cut	2181B130717	10
Klenk	Peppermint leaf, cut	2181A101013	6
Klenk	Peppermint leaf, cut	2161A111207	1
Klenk	Peppermint leaf, cut	2181A120913	33

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Supplier	Substance	Batch	Spectra
Klenk	Peppermint leaf, cut	2161B140321	1
Klenk	Peppermint leaf, cut	2161	1
Klenk	Peppermint leaf, cut	2181A130320	6
Klenk	Peppermint leaf, cut	2181A100323	1
Klenk	Peppermint leaf, cut	2181A151119	1
Klenk	Peppermint leaf, cut	1001311505	1
Klenk	Peppermint leaf, cut	1209211505	1
Klenk	Peppermint leaf, cut	A121009	1
Klenk	Peppermint leaf, cut	2181A-101013	1
Klenk	Peppermint leaf, cut	2181a120913	3
Klenk	Peppermint leaf, cut	2161A07020203	1
Klenk	Peppermint leaf, cut	2161A121206	14
Klenk	Primrose flower	1540A-100907	1
Klenk	Primrose flower	B130808	1
Klenk	Primrose flower	1541B100414	1
Klenk	Primrose flower	1540A100907	1
Klenk	Primrose flower	B110314	1
Klenk	Primrose flower	1541B110314	7
Klenk	Primrose flower	A111018	1
Klenk	Primrose flower	B130808	1
Klenk	Primrose root, cut	B130218	3
Klenk	Primrose root, cut	6461A100511	1
Klenk	Psyllium seed	7380A111018	1
Klenk	Psyllium seed	7380A130128	6
Klenk	Psyllium seed	7380A110317	1
Klenk	Psyllium seed	7380A120109	22
Klenk	Psyllium seed	A130128	1
Klenk	Psyllium seed	A120109	1
Klenk	Psyllium seed	7380a111018	1
Klenk	Psyllium seed	7380A150520	4
Klenk	Psyllium seed	7380a120109	3
Klenk	Psyllium seed	7560A130418	1
Klenk	Psyllium seed	7560a120330	1
Klenk	Psyllium seed	7380A120911	16
Klenk	Psyllium seed	A120911	1
Klenk	Psyllium seed	7560A140203	1
Klenk	Ramsons herb, cut	3511B111005	2
Klenk	Raspberry leaf, cut	2291A111124	1
Klenk	Raspberry leaf, cut	2291a111124	1
Klenk	Raspberry leaf, cut	2291A120507	5
Klenk	Raspberry leaf, cut	12273107	1
Klenk	Raspberry leaf, cut	2291A121120	4
Klenk	Raspberry leaf, cut	2291A130320	1
Klenk	Raspberry leaf, cut	A130430	1
Klenk	Raspberry leaf, cut	2291A110125	1
Klenk	Raspberry leaf, cut	2291A120813	1
Klenk	Red clover flower	1640a130122	1
Klenk	Red clover flower	1640A110727	1
Klenk	Red clover flower	1640A130122	13
Klenk	Red clover flower	7470A130311	1
Klenk	Red clover flower	811Q-07163	1
Klenk	Red-rose petal	1561A121016	1
Klenk	Red-rose petal, cut	1561A110404	1
Klenk	Red-rose petal, cut	1561B101210	2
Klenk	Red-rose petal, cut	1561A121016-34023101	1
Klenk	Redwood	5961B111219	1
Klenk	Restharrow root, cut	B111110	1
Klenk	Restharrow root, cut	6411B101216	2
Klenk	Restharrow root, cut	4296345	1
Klenk	Restharrow root, cut	6411111110	1

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Supplier	Substance	Batch	Spectra
Klenk	Restharrow root, cut	6411B130404	2
Klenk	Restharrow root, cut	6411B111110	1
Klenk	Rhubarb, cut	7761B130514	2
Klenk	Rhubarb, cut	6891B111118	1
Klenk	Ribwort plantain, cut	A110816	1
Klenk	Ribwort plantain, cut	4281N111121	1
Klenk	Ribwort plantain, cut	427A111125	1
Klenk	Ribwort plantain, cut	4271A130716	1
Klenk	Ribwort plantain, cut	4271A111125	2
Klenk	Ribwort plantain, cut	4271A130115	6
Klenk	Ribwort plantain, cut	4271A100615	2
Klenk	Ribwort plantain, cut	4271A110816	2
Klenk	Ribwort plantain, cut	4271A-110816	1
Klenk	Robert herb, cut	3951B12118	1
Klenk	Robert herb, cut	3951A110621	6
Klenk	Robert herb, cut	A110621	6
Klenk	Robert herb, cut	3951B121218	2
Klenk	Rose hips peel, cut	2851A-110202	1
Klenk	Rose hips peel, cut	2841B111019	2
Klenk	Rose hips peel, cut	2851A120102	5
Klenk	Rose hips peel, cut	2851A110202	1
Klenk	Rose hips peel, cut	2851A120904	2
Klenk	Rose hips peel, cut	3613M-01543	1
Klenk	Rose hips peel, cut	A120904	3
Klenk	Rose hips peel, cut	2851A101119	3
Klenk	Rose hips peel, cut	2851A150310	4
Klenk	Rose hips with peel, ...	B130523	1
Klenk	Rose hips with peel, ...	A120719	1
Klenk	Rose hips with peel, ...	3613M-01542	1
Klenk	Rose hips with peel, ...	2841B081210	1
Klenk	Rose hips with peel, ...	2841B111019	3
Klenk	Rose hips with peel, ...	B111019	1
Klenk	Rose hips with peel, ...	2851A120904	1
Klenk	Rose hips with peel, ...	A120904	1
Klenk	Roselle	1431B130205	1
Klenk	Roselle	1431B-110519	1
Klenk	Roselle	1431B131015	2
Klenk	Roselle	1431B111122	1
Klenk	Roselle	B130205	1
Klenk	Rosemary leaf, cut	2261A131118	12
Klenk	Rosemary leaf, cut		1
Klenk	Rosemary leaf, cut	61A131118	1
Klenk	Rosemary leaf, cut	2261A140910	3
Klenk	Rosemary leaf, cut	2261A150622	5
Klenk	Rosemary leaf, cut	2261A120224	18
Klenk	Rosemary leaf, cut	2261A160329	1
Klenk	Rosemary leaf, cut	2261a160329	1
Klenk	Rosemary leaf, cut	2261A081117	1
Klenk	Rosemary leaf, cut	112E-01510	1
Klenk	Rosemary leaf, cut	2261A130201	29
Klenk	Rosemary leaf, cut	2261A160905	2
Klenk	Rosemary leaf, cut	2261a120224	2
Klenk	Rosemary leaf, cut	301401	1
Klenk	Rosemary leaf, cut	A130201	2
Klenk	Rue herb, cut	A120207	1
Klenk	Rue herb, cut	4361A120207	1
Klenk	Rue herb, cut	4361A07020601	1
Klenk	Rue herb, cut	4361A100707	3
Klenk	Saffron (spice)	384A-120410	1
Klenk	Saffron (spice)	384a120410	1

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Supplier	Substance	Batch	Spectra
Klenk	Saffron (spice)	384A130320	2
Klenk	Saffron (spice)	384A110608	1
Klenk	Saffron filaments	380A130613	1
Klenk	Sage leaf, cut	2301C12026	1
Klenk	Sage leaf, cut	2301a120403	1
Klenk	Sage leaf, cut	2301A110420	1
Klenk	Sage leaf, cut	2301C120126	15
Klenk	Sage leaf, cut	C120126	1
Klenk	Sage leaf, cut	2301A110420	2
Klenk	Sage leaf, cut	2301c120126	1
Klenk	Sage leaf, cut	2301C12126	1
Klenk	Sarsaparilla root, cut	6561B111108	1
Klenk	Sarsaparilla root, cut	B111108	1
Klenk	Senna leaf, cut	2331B150903	1
Klenk	Senna leaf, cut	2331B130214	3
Klenk	Senna leaf, cut	2331B120403	1
Klenk	Senna leaf, cut	2331A110207	1
Klenk	Senna leaf, cut	2331A100525	2
Klenk	Senna leaf, cut	B130214	1
Klenk	Senna leaf, cut	2331B110907	2
Klenk	Senna leaf, cut	2331C120614	8
Klenk	Senna leaf, cut	2331c130326	1
Klenk	Senna leaf, cut	2331C130326	16
Klenk	Senna pods, tinnevelly	1041B120327	2
Klenk	Shepherd's purse, cut	3671A-100414	2
Klenk	Shepherd's purse, cut	B111201	1
Klenk	Shepherd's purse, cut	3671B111201	1
Klenk	Silverweed, cut	11328103	4
Klenk	Silverweed, cut	H-280513-3	1
Klenk	Silverweed, cut	A110913	2
Klenk	Silverweed, cut	3551A130903	1
Klenk	Solanum dulcamara ste...	5601A080513	3
Klenk	St. John's wort, cut	A121120	1
Klenk	St. John's wort, cut	A130612	3
Klenk	St. John's wort, cut	4021a120604	1
Klenk	St. John's wort, cut	4021A130612	3
Klenk	St. John's wort, cut	15068103	2
Klenk	St. John's wort, cut	4021A120905	8
Klenk	St. John's wort, cut	4021A100819	1
Klenk	St. John's wort, cut	4021A120604	15
Klenk	St. John's wort, cut	4021A100819914	2
Klenk	St. John's wort, cut	4021B110321	2
Klenk	St. John's wort, cut	4021A100819	21
Klenk	St. John's wort, cut	4021A100919	1
Klenk	St. John's wort, cut	4021A00819	1
Klenk	St. John's wort, cut	4021a100819	1
Klenk	Star anise	2690A101026	1
Klenk	Star anise	2690A120809	1
Klenk	Star anise	2690A111013	3
Klenk	Star anise	2696B111109	1
Klenk	Star anise	2690A130903	2
Klenk	Star anise	B111109	1
Klenk	Stemless carline root	6194b110831	1
Klenk	Stemless carline root	B110831	1
Klenk	Stemless carline root	69191B120726	1
Klenk	Stemless carline root	6191B120726	3
Klenk	Stemless carline root	6194B110831	1
Klenk	Stemless carline root	12097301	1
Klenk	Strawberry leaf, cut	2031B110224	2
Klenk	Strawberry leaf, cut	B120925	1

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Supplier	Substance	Batch	Spectra
Klenk	Strawberry leaf, cut	2031A130430	2
Klenk	Strawberry leaf, cut	A130430	1
Klenk	Sunflower, cut	1711I-07036	1
Klenk	Sunflower, cut	1701B091013	1
Klenk	Sweet fennel	2870130304A	1
Klenk	Sweet fennel	2870A140528	1
Klenk	Sweet fennel	2870A131002	1
Klenk	Sweet woodruff herb, ...	3601B140321	1
Klenk	Sweet woodruff herb, ...	3601B090114	1
Klenk	Sweet woodruff herb, ...	B090114	3
Klenk	Tall golden rod, cut	A110209	1
Klenk	Tall golden rod, cut	4521A-110816	1
Klenk	Tall golden rod, cut	4521A100414	1
Klenk	Tall golden rod, cut	4521A110209	3
Klenk	Tall hawkweed, cut	B111005	1
Klenk	Tall hawkweed, cut	3611B11105	1
Klenk	Theriac, powdered	12189403	1
Klenk	Thyme, rubbed	4622A110728	25
Klenk	Thyme, rubbed	4622a110728	1
Klenk	Thyme, rubbed	1910211688	1
Klenk	Thyme, rubbed	4622B110519	1
Klenk	Thyme, rubbed	4622A141203	1
Klenk	Thyme, rubbed	A130910	3
Klenk	Thyme, rubbed	4622a130109	2
Klenk	Thyme, rubbed	4622A120111	34
Klenk	Thyme, rubbed	2103311688	1
Klenk	Thyme, rubbed	4622A130910	2
Klenk	Thyme, rubbed	4622A-120111	1
Klenk	Thyme, rubbed	4622a120111	3
Klenk	Tormentil	6911B131029	4
Klenk	Tormentil	6911B111013	10
Klenk	Tormentil	6911B150825	4
Klenk	Tormentil	6911B141114	1
Klenk	Tormentil	6914b120112	1
Klenk	Tormentil	6911B140227	1
Klenk	Turmeric root, cut	6741B121030	1
Klenk	Turmeric, javanese, cut	B130117	1
Klenk	Turmeric, javanese, cut	6731B150630	1
Klenk	Valerian root, cut	6641B100823	1
Klenk	Valerian root, cut	13196808	1
Klenk	Valerian root, cut	6645B130226	1
Klenk	Valerian root, cut	6641B130226	9
Klenk	Valerian root, cut	6641B-110317	1
Klenk	Valerian root, cut	6641B120417	1
Klenk	Valerian root, cut	6641B110317	2
Klenk	Verbena herb, cut	4651B130611	2
Klenk	Verbena herb, cut	4651A070828	3
Klenk	Verbena herb, cut	4654B120611	1
Klenk	Verbena herb, cut	4651B120611	16
Klenk	Verbena herb, cut	A130923	1
Klenk	Walnut bark, cut	711b120613	1
Klenk	Walnut bark, cut	711B080806	1
Klenk	Walnut bark, cut	711B120906	1
Klenk	Walnut bark, cut	711B120613	3
Klenk	Walnut leaf, cut	A130410	1
Klenk	Walnut leaf, cut	2111A130410	2
Klenk	Walnut leaf, cut	F-280513-1	1
Klenk	Walnut leaf, cut	2111A110816	1
Klenk	Walnut leaf, cut	2111A131029	1
Klenk	Walnut leaf, cut	2111A-120123	1

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Supplier	Substance	Batch	Spectra
Klenk	White deadnettle flower	1470A080103	1
Klenk	White deadnettle flower	1470A120111	4
Klenk	White mustard seed, p...	7254A141202	1
Klenk	Wild pansy, cut	4681B130715	5
Klenk	Wild pansy, cut	B130715	1
Klenk	Wild pansy, cut	4681A120806	15
Klenk	Wild pansy, cut	4681A110303	2
Klenk	Wild pansy, cut	4681A-120806	1
Klenk	Willow bark, cut	811B100910	3
Klenk	Willow bark, cut	B100910	6
Klenk	Willowherb, small flo...	4721A101010	2
Klenk	Willowherb, small flo...	4721C110701	4
Klenk	Willowherb, small flo...	4721A120418	10
Klenk	Willowherb, small flo...	4721C120321	10
Klenk	Willowherb, small flo...	A120418	1
Klenk	Willowherb, small flo...	4721A120903	7
Klenk	Willowherb, small flo...	4721C2120321	1
Klenk	Willowherb, small flo...	2512U-01641	1
Klenk	Willowherb, small flo...	4721C130618	4
Klenk	Willowherb, small flo...	4721B130528	1
Klenk	Willowherb, small flo...	C120321	1
Klenk	Wormwood herb, cut	3461A1100324	1
Klenk	Wormwood herb, cut	3461A121130	2
Klenk	Wormwood herb, cut	A110324	1
Klenk	Wormwood herb, cut	3461A110324	2
Klenk	Yarrow flower, rubbed	4181A121130	1
Klenk	Yarrow flower, rubbed	A110816	3
Klenk	Yarrow herb, cut	4181130709	1
Klenk	Yarrow herb, cut	4181a130513	1
Klenk	Yarrow herb, cut	15333007	1
Klenk	Yarrow herb, cut	4181A121130	12
Klenk	Yarrow herb, cut	4181A110111	15
Klenk	Yarrow herb, cut	4181A101102	1
Klenk	Yarrow herb, cut	4181A130710	1
Klenk	Yarrow herb, cut	4181a11011	1
Klenk	Yarrow herb, cut	4181B130709	2
Klenk	Yarrow herb, cut	A130709	1
Klenk	Yellow chaste weed, cut	1591A-110511	1
Klenk	Yellow chaste weed, cut	1591A110511	12
Klenk	Zedoary root, cut	6941B121025	3
Klenk	Zedoary root, cut	6941B110329	2
Klenk	Zedoary root, powdered	12007505	1
Kottas	Bitter fennel	P15301479	1
kräuter schulte	Bitter orange peel, cut	51265	1
kräuter schulte	Gentian root, cut	52348	1
kräuter schulte	Red-rose petal, cut	47543	1
kräuter schulte	Tormentil	51952	1
Kräuter Schulte	Black cohosh, cut	3308M-02176	1
Kräuter Schulte	Blackthorn flower, ru...	53233	2
Kräuter Schulte	Bucho leaf	54519	1
Kräuter Schulte	China Pai Mu Tan	52783	1
Kräuter Schulte	Couch grass rhizome, ...	53016	2
Kräuter Schulte	Dill fruit	6363	1
Kräuter Schulte	Dryas octopetala herb...	38970	1
Kräuter Schulte	Geum urbanum herb, cut	51737	1
Kräuter Schulte	Meadowsweet flower, r...	51369	1
Kräuter Schulte	Meadowsweet flower, r...	53473	1
Kräuter Schulte	Red clover flower	53778	1
Kräuter Schulte	Red tea	52029	1
Kräuter Schulte	Saponaria root, cut	54500	1

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Supplier	Substance	Batch	Spectra
Kräuter Schulte	Saponaria root, cut	54524	2
Kräuter Schulte	Saponaria root, cut	54977	1
Kräuter-Schulte	Peppermint leaf, cut	56254	1
Kräuter-Schulte	Sorrel herb, cut	55272	1
Kräuter-Schulte	Sweet woodruff herb, ...	52878	1
Macfarlan Smith/Noweda	Cocaine hydrochloride	15224802	2
Macsen laboratories/P...	Methylrosanilinium ch...	1989	1
Merck	Codeine phosphate hem...	120765	1
Merck	Heavy alkaline bismut...	75419201	1
Merck	Trichloroacetic acid	12821	1
Nachprüfung	Abrotani herb, cut	3451A070919	1
Nachprüfung	Aniseed	5010U-01530	1
Nachprüfung	Black cohosh, cut	10281113	1
Nachprüfung	Blackcurrant leaf, cut	1003	1
Nachprüfung	Fenugreek, powdered	2412E02239	1
Nachprüfung	Ginkgo leaf, cut	2461A100429	9
Nachprüfung	Hay flower	1911E01459	1
Nachprüfung	Heather, cut	5110A03224	1
Nachprüfung	Stemless carline root	2812U02133	1
Nachprüfung	Wild pansy, cut	10291007	1
noweda	Dandelion root, cut		1
noweda	Iceland moss, cut		1
noweda	Walnut leaf, cut		1
Noweda	Abrotani herb, cut	3451A120312	18
Noweda	Agrimony, cut	10325503	2
Noweda	Agrimony, cut	9300106	1
Noweda	Alchemilla, cut	12153302	13
Noweda	Amphetamine sulfate	16A29-B03-318744	3
Noweda	Angelica root	272720	2
Noweda	Bentonite	11304415	1
Noweda	Caffeine citrate	CCC-1101	1
Noweda	Calendula flower, cut	12221709	9
Noweda	Caraway fruit	12226605	3
Noweda	Caraway fruit	12226503	6
Noweda	Coltsfoot leaf, cut	2021B111111	3
Noweda	Damiana leaf, cut	200151	1
Noweda	Elecampane rhizome, cut	6341B111118	3
Noweda	Equisetum stem, cut	12231401	6
Noweda	Heavy alkaline bismut...	13/01-N02	1
Noweda	Hop strobile	274725	1
Noweda	Linseed	7307A111107	7
Noweda	Liquorice root, peeled	70226/1	1
Noweda	Manna, powdered	11170102	1
Noweda	Marjoram herb, rubbed	4881A100929	3
Noweda	Marrubium vulgare her...	4141A080513	1
Noweda	Methylrosanilinium ch...	12H28-N06	1
Noweda	Methylrosanilinium ch...	2159	2
Noweda	Mistletoe, cut	11294001	1
Noweda	Molecular distilled g...	11160010	1
Noweda	Nettle leaf, cut	12195001	6
Noweda	Oak bark, cut	10348617	8
Noweda	Oat straw, cut	11280003	1
Noweda	Peppermint leaf, cut	2911U-01505	1
Noweda	Potassium hydrocarbon...	1004019-01	1
Noweda	Primrose root, cut	12064504	4
Noweda	Rosemary leaf, cut	15428011	1
Noweda	Rosemary leaf, cut	2261A100916	1
Noweda	Salbutamol sulfate	13K12-N02	1
Noweda	St. John's wort, cut	12092202	6
Noweda	Stemless carline root	12163702	1

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Supplier	Substance	Batch	Spectra
Noweda	Tall golden rod, cut	11280306	3
Noweda	Thyme, rubbed	521303908	1
Noweda	Tonka beans	1040A111026	1
Noweda	Tragacanth, powdered	14162207	1
Noweda	Willow bark, cut	4609A-01305	1
Noweda	Yarrow herb, cut	13381804	2
Noweda	Yarrow herb, cut	12378603	1
Noweda	Zedoary root, cut	11091605	3
Noweda / 28.10.13 EuRho	Magnesium sulfate hep...	1211022-01	3
Noweda 06.04.2016	Bitter fennel	15443201	1
Noweda/Henry Lamotte	Black mustard seed, p...	1493708	1
Noweda/10.02.2017	Tormentil	15364313	1
Phagron	Yarrow herb, cut		3
Phoenix	Centaury, cut	11097612	9
Phoenix	Fenugreek	11313206	6
Phoenix	Gentian root, cut	6311B120104	1
Phoenix	Juniper		1
Phoenix	Liquorice root, peeled	6381A120611	12
Phoenix	Raspberry leaf, cut	10136409	1
Phoenix	Rhubarb, cut	11057817	3
Phoenix	Ribwort plantain, cut	4271A11016	1
Phoenix	Sage leaf, cut	231C130326	1
Phoenix	Talcum	1305022-01	1
Phoenix	Wormwood herb, cut	12103003	8
PHOENIX 19.05.2014	Black pepper	13221105	1
PHOENIX am 27.12.2013	Liquorice root, natur...	281844	1
Phonix	Linseed	13296703	3
phönix	Aloes, cape, cut	15283011	1
phönix	Methylrosanilinium ch...	13184811	1
phönix	Myrrh	15021411	1
phönix	Myrrh	3351a160330	1
phönix	Sodium alginate	11509036-02	1
phönix	Tormentil	15364343	1
Phönix	Amphetamine sulfate	16a29-b03-328317	1
Phönix	Amphetamine sulfate	13B11N04	1
Phönix	Bitter fennel	12094708	2
Phönix	Centaury, cut	11093612	2
Phönix	Cinchocaine hydrochlo...	13E13-N07	1
Phönix	Cinnamon rods (Ceylon...	610A130927	1
Phönix	Coltsfoot leaf, cut	278296	3
Phönix	Common broom herb, cut	12358801	2
Phönix	Creatine	mysjhskeu	1
Phönix	Dandelion herb with r...	6611B130321	27
Phönix	Equisetum stem, cut	12288807	2
Phönix	Gentian root, cut	6311B120315	7
Phönix	Gentian root, cut	269197	2
Phönix	Ginger, peeled	13310601	1
Phönix	Ground ivy herb, cut	11374608	1
Phönix	Hyssop herb, cut	11374306	1
Phönix	Iceland moss, cut	12187104	3
Phönix	Ivy leaf, cut	11101102	1
Phönix	Jasmine flower	12143206	1
Phönix	Juniper	13020903	1
Phönix	Lime flower, cut	1611A12120	1
Phönix	Lime flower, cut	2090413	1
Phönix	Liquorice root, natur...	276425	1
Phönix	Male speedwell wort, ...	13089201	4
Phönix	Marshmallow root, pee...	6071a120314	1
Phönix	Marshmallow root, pee...	6071A130408	13
Phönix	Marshmallow root, pee...	2090413	1

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Supplier	Substance	Batch	Spectra
Phönix	Matricaria flower	1300A120426	1
Phönix	Melilot herb, cut	1237903	1
Phönix	Methadone hydrochloride	16135309	2
Phönix	Motherwort herb, cut	12231503	1
Phönix	Oak bark, cut	10348609	2
Phönix	Peppermint leaf, cut	11327808	2
Phönix	Raspberry leaf, cut	12362701	7
Phönix	Rhubarb, cut	12211905	3
Phönix	Rose hips with peel, ...	10281021	1
Phönix	Rose hips with peel, ...	2841B130523	1
Phönix	Rose hips with peel, ...	2841B130523	1
Phönix	Silverweed, cut	11328107	7
Phönix	Sodium carbonate deca...	13036904	2
Phönix	Sodium hydrogen carbo...	13186705	3
Phönix	Sodium hydrogen carbo...	13390515	1
Phönix	Sodium monohydrogenph...	1302800,	1
Phönix	Sodium monohydrogenph...	13028101	1
Phönix	Tormentil	15364302	1
Phönix	Wormwood herb, cut	12355806	6
Phönix	Yarrow herb, cut	4181A130513	8
Phönix 10.01.2014	Senna leaf, cut	13136707	1
Phönix/Euro	Magnesium chloride he...	1208025-01	2
Probe	Elder root, cut	12345	1
Probe	Peppermint leaf, cut	1223456	1
Purren Apotheke	Heavy alkaline bismut...	11H31-N06	1
Redwood	Damiana leaf, cut	216451	1
Richter	Common wormwood herb,...	b200112	1
Richter	Elecampane rhizome, cut	P158683	1
Richter	Gentian root, cut	P200907	1
Richter	Ginger, peeled	KR27992	1
Richter	Ground ivy herb, cut	s99/09	1
Richter	Horse chestnut flower. ...	s-09/09	1
Richter	Lungwort herb, cut	P195884	1
Richter	Maize style, cut	B189316	1
Richter	Red-rose petal, cut	P236157	1
Richter	Tormentil	P209904	1
Rondell Apotheke	Caffeine citrate	15A05-B03-307309	2
sana 09.12.14 3,75	Guaiacum wood, cut	13343802	1
Sana 21.10.14 Ek 3.57	Maize style, cut	13381603	2
sanacorp	Caraway fruit	2656259	1
sanacorp	Pumpkin seed, peeled	14186909	1
Sanacorp	Agnus castus fruit	12274006	3
Sanacorp	Alchemilla, cut	12153309	14
Sanacorp	Aluminium potassium s...	12184402	2
Sanacorp	Amphetamine sulfate	12/24-N03	1
Sanacorp	Angelica root	277310	1
Sanacorp	Bearberry leaf, cut	2391B110209	3
Sanacorp	Betony herb, cut	13048903	3
Sanacorp	Bilberry leaf, cut	2191A130410	2
Sanacorp	Blackcurrant leaf, cut	2251A110204	4
Sanacorp	Calendula flower, cut	12221601	4
Sanacorp	Caraway fruit	2770A120905	4
Sanacorp	Caraway fruit		2
Sanacorp	Chicory herb, cut	12369101	5
Sanacorp	Cinnamon rods (Ceylon...	13231601	1
Sanacorp	Dandelion herb with r...	13108803	2
Sanacorp	Equisetum stem, cut	13344307	1
Sanacorp	European golden rod, ...	12343103	1
Sanacorp	Feverfew herb, cut	12380201	2
Sanacorp	Goat's rue, cut	12017911	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Heavy alkaline bismut...	12146909	2
Sanacorp	Hyssop herb, cut	11374303	1
Sanacorp	Hyssop herb, cut	13336101	6
Sanacorp	Juniper	12330509	1
Sanacorp	Kelp, cut	11351105	1
Sanacorp	Ladys bedstraw herb,...	12369003	8
Sanacorp	Ladys bedstraw herb,...	11265109	1
Sanacorp	Lime flower, cut	264045	1
Sanacorp	Liquorice root, peeled	11351906	3
Sanacorp	Lycopodium herb, cut	13101502	2
Sanacorp	Mallow leaf, cut	278925	1
Sanacorp	Matricaria flower	1290B140123	2
Sanacorp	Matricaria flower	12294804	6
Sanacorp	Matricaria flower	1300A120725	2
Sanacorp	Matricaria flower	12294809	3
Sanacorp	Meadowsweet herb, cut	4541A120313	2
Sanacorp	Methadone hydrochloride	12171913	1
Sanacorp	Methadone hydrochloride	12344806	2
Sanacorp	Morphine hydrochloride	18188601	1
Sanacorp	Morphine hydrochloride	16184605	1
Sanacorp	Morphine hydrochloride	16184612	2
Sanacorp	Nettle leaf, cut	12184003	17
Sanacorp	Nettle leaf, cut	12184707	11
Sanacorp	Nettle root, cut	11265001	2
Sanacorp	Nettle seed	13010602	1
Sanacorp	Orris root	11026701	1
Sanacorp	Primrose flower	1541B130808	6
Sanacorp	Pumpkin seed, peeled	16081212	1
Sanacorp	Raspberry leaf, cut	13038001	6
Sanacorp	Raspberry leaf, cut	12362703	9
Sanacorp	Ribwort plantain, cut	263401	1
Sanacorp	Roselle	12267508	2
Sanacorp	Senna leaf, cut	13136701	4
Sanacorp	Tormentil	12040712	3
Sanacorp	Valerian root, cut	12033804	9
Sanacorp	Wild pansy, cut	12221-01694	1
Sanacorp	Wormwood herb, cut	12103002	2
sanacorp;3,32;18.06.15	Coriander	13299495	1
Siegfried Ltd	Methadone hydrochloride	12B21-N03	1
Siegfried Ltd, Divisi...	Methadone hydrochloride	15244712	1
siehe Protokoll	Aniseed	sieheProtokoll	1
siehe Protokoll	Cinnamon, cut	sieheProtokoll	1
siehe Protokoll (Galke)	Bitter fennel	sieheProtokoll	2
siehe WE-Prüfprotokoll	8-quinolinol sulfate ...	96/09	1
Sigma-Aldrich	Sodium butyrate	Lot.091M-5302V	1
Sigma-Aldrich	Sodium propionate	SLBK5249V	1
Sino Phyto	Agrimony, cut	12382905	5
Spangro/gepepharm	Bitter fennel	15007602	2
Spangropharm	Birch leaf, cut	264603	1
Spangropharm	Matricaria flower	11169606	1
Spangropharm	Mistletoe, cut	10273408	1
Spinnrad	Black cumin seed	11931059	1
Spinnrad/Phoenix	Black cumin seed	613310592	1
stumpf	Magnesium chloride he...	1301c012-277804	1
Synop	Morphine hydrochloride	15I09-B08	1
Synopharm	Cocaine hydrochloride	16B11-B05	1
Th. Geyer	Amphetamine sulfate	67043	52
Th. Geyer	Amphetamine sulfate	20170808-03361	1
Th. Geyer	Amphetamine sulfate	57043	1
Th. Geyer	Amphetamine sulfate	67002	45

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Th. Geyer	Amphetamine sulfate	21082013B	1
Th. Geyer	Amphetamine sulfate	L0T067043	1
Th. Geyer	Amphetamine sulfate	PH10051	1
Th. Geyer	Amphetamine sulfate	70325	2
Th. Geyer	Codeine phosphate hem...	67038	1
Th. Geyer	Codeine phosphate hem...	67054	31
Th. Geyer	Dihydrocodeine hydrog...	59819	1
Th. Geyer	Dihydrocodeine hydrog...	67035	2
Th. Geyer	Dihydrocodeine hydrog...	20170808-03065	1
Th. Geyer	Dihydrocodeine hydrog...	67052	10
Th. Geyer	Methadone hydrochloride		1
Th. Geyer	Methadone hydrochloride	70246	1
Th. Geyer	Methadone hydrochloride	70245	38
Th. Geyer	Methadone hydrochloride	67055	10
Th. Geyer	Methadone hydrochloride	67047	2
Th. Geyer	Morphine hydrochloride	2615M-01879	1
Th. Geyer	Morphine hydrochloride	67036	5
Th. Geyer	Morphine hydrochloride	PH120087	1
Th. Geyer	Morphine hydrochloride	1415E-01879	1
Th. Geyer	Phenobarbital	67045	2
unbekannt	Magnesium chloride he...	unbekannt	1
Unisan	D-ribose	JXCZSJ13D-013	2
Unisan	Sodium sulfate decahy...	11294605	1
VDL	Basil, rubbed	12007004	1
VDL	Boldo leaf, cut	11016503	1
VDL	Eucalyptus leaf, cut	2011B110801	4
VDL	Java tea, cut	2221B101213	1
VDL	Primrose flower	11206806	1
VDL	Raspberry leaf, cut	10013406	3
VDL	Yellow chaste weed, cut	10244406	1
VDL;15.06.15;6,83EUR	Caraway fruit	13306007	1
VDL;87,00EUR;08.09.14	Methadone hydrochloride	12344821	1
vedono	Aniseed, powdered	11306208	1
vedono	Frankincense	12120009	5
vedono	Frankincense	12120012	1
vedono	Hawthorn leaf with fl...	12225103	4
vedono	Rhubarb, cut	12211907	6
vedono	Roselle	12007313	1
vedono	Wild thyme, cut	11374807	2
vedono	Zedoary root, cut	13010106	3
Weltecke	Angelica root	38011111	1
Weltecke	Meadowsweet herb, cut	67010413	1
Weltecke	Thyme, rubbed	67101212	1
Weltecke / GEHE	Primrose flower	63011112	1
Wolf	Alchemilla, cut	p931	1
Wolf	Alchemilla, cut	B-698	2
Wolf	Alchemilla, cut	23187	4
Wolf	Alchemilla, cut	E-822	1
Wolf	Aniseed	216346	1
Wolf	Aniseed	B216346	14
Wolf	Aniseed	L401F1413	1
Wolf	Aniseed	L401F292b	4
Wolf	Aniseed	B671	1
Wolf	Aniseed	B-671	2
Wolf	Aniseed	215346	1
Wolf	Bitter fennel	B362	2
Wolf	Bitter fennel	B-493	1
Wolf	Bitter fennel	B-682	1
Wolf	Bitter fennel	B382	1
Wolf	Bitter fennel	B492	1

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Supplier	Substance	Batch	Spectra
Wolf	Bitter fennel	B-492	5
Wolf	Bitter fennel	B-362	1
Wolf	Black cumin seed	20720	8
Wolf	Black cumin seed	207204	1
Wolf	Black cumin seed	L402F1713	1
Wolf	Black cumin seed	L402F171b	3
Wolf	Black cumin seed	B-471	1
Wolf	Black cumin seed	L310F141b	6
Wolf	Black cumin seed		1
Wolf	Calendula flower	23342	1
Wolf	Caraway fruit	B-224	1
Wolf	Dill fruit	E-501	1
Wolf	Dill fruit	23622	6
Wolf	Dill fruit	L30057	5
Wolf	Elder flower, rubbed	22749	1
Wolf	Elder flower, rubbed	22765	1
Wolf	Elder flower, rubbed	B-810	1
Wolf	Elder flower, rubbed	E-738	1
Wolf	Equisetum stem, cut	B-695	1
Wolf	Equisetum stem, cut	B233885	4
Wolf	Lemon grass, cut	B654	1
Wolf	Lemon verbena leaf, cut	23635	1
Wolf	Lemon verbena leaf, cut	B-312	1
Wolf	Lemon verbena leaf, cut	E-587	1
Wolf	Lime flower, cut	22094	1
Wolf	Lime flower, cut	B449	1
Wolf	Marjoram herb, rubbed	163516	1
Wolf	Marjoram herb, rubbed	P232243	9
Wolf	Marjoram herb, rubbed	B163516	6
Wolf	Matricaria flower	23242	1
Wolf	Nettle leaf, cut	B-821	1
Wolf	Nettle leaf, cut	P234605	10
Wolf	Nettle leaf, cut	B821	1
Wolf	Peppermint leaf, cut	B725	1
Wolf	Peppermint leaf, cut	P221379	7
Wolf	Peppermint leaf, cut	B-120	1
Wolf	Peppermint leaf, cut	B243	1
Wolf	Peppermint leaf, cut	B-725	2
Wolf	Raspberry leaf, cut	B-457	1
Wolf	Raspberry leaf, cut	P201727	19
Wolf	Raspberry leaf, cut	P222676	1
Wolf	Sage leaf, cut	B735	1
Wolf	Shepherd's purse, cut	B449	2
Wolf	St. John's wort, cut	B-455	2
Wolf	St. John's wort, cut	19468	2
Wolf	St. John's wort, cut	206152	1
Wolf	St. John's wort, cut	B206152	1
Wolf	St. John's wort, cut	B-424	1
Wolf	Yarrow herb, cut	230010	1
Wolf	Yarrow herb, cut	B230010	9
-	Angelica root	130924	1
-	Bitter orange flower ...	2011A-01445	1
-	Burdock root, cut	5110I-02131	1
-	Chelidonium majus her...	810I-01632	1
-	Chickweed, cut	2011A-01686	1
-	Chicory herb, cut	4411I-01634	1
-	Elecampane rhizome, cut	712M-02181	1
-	Gentian root, powdered	130063	1
5N Plus Lübeck GmbH/ ...	Heavy alkaline bismut...	12146908	1
-	Iceland moss, cut	4711E-01774	1

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Supplier	Substance	Batch	Spectra
-	Meadowsweet herb, cut	130849	1
-	Meadowsweet herb, cut	1511M-01685	1
-	Melilot herb, cut	811Q-01664	1
-	Melissa leaf, cut	131146	1
-	Raspberry leaf, cut	130849	1
-	Silverweed, cut	711M-01619	1
-	Silverweed, cut	130849	1
-	Wild thyme, cut	131023	1
-	Wild thyme, cut	130685	1

Appendix D: Requirements of validation

In order to ensure adherence to the safe scientific status, the individual methods for manufacturing and testing must be validated under certain circumstances (compare § 34 para. 1 no. 3, § 35 para. 1 no. 4 and para. 4 sentence 1 no. 2 b, para. 6 sentence 3 *ApoBetrO* [Pharmacies Rules and Regulations]). The *ApoBetrO* [Pharmacies Rules and Regulations] incorporates a legal definition in § 1 a para. 16 (quotation translated):

“Validation is the provision of documented proof which with a high degree of safety documents that, via a specific process or standard work process, a medicinal product is manufactured and tested, which is in accordance with previously determined quality features.”

Validation documentation can be used to prove that methods or devices which are not described in the Pharmacopoeia within the meaning of § 6 para. 1 sentence 3 *ApBetrO* [Pharmacies Rules and Regulations] achieve the same results as those in the Pharmacopoeia. On the other hand, with the requirements of the demanded validation it must be observed whether the respective testing method is already incorporated in the Pharmacopoeia.

NIR spectroscopy as a general testing method need not be validated in accordance with the express ruling in the *Ph. Eur. Section 1.1* [3], as it is already described in *Section 2.2.40* of the *Ph. Eur.* as an area of application for the identification of raw materials.

However, a special validation requirement exists for the reference database. This requirement is met with the existing document. Further requirements or rules as to how this proof must be furnished do not exist. It is required that the processes guarantee the same results as the methods and devices in the Pharmacopoeia [17].

Carrying out identity tests with *Apo-Ident* is therefore also possible if the NIR spectroscopy process is not required in the Pharmacopoeia monograph of the substance for identity testing. All NIR analyses with *Apo-Ident* prove several, often all molecule groups and are therefore comparable with a series of individual, targeted chemical proofs [4]. Therefore, the identity proof with *Apo-Ident* replaces the monograph test series (with two or more test combinations).

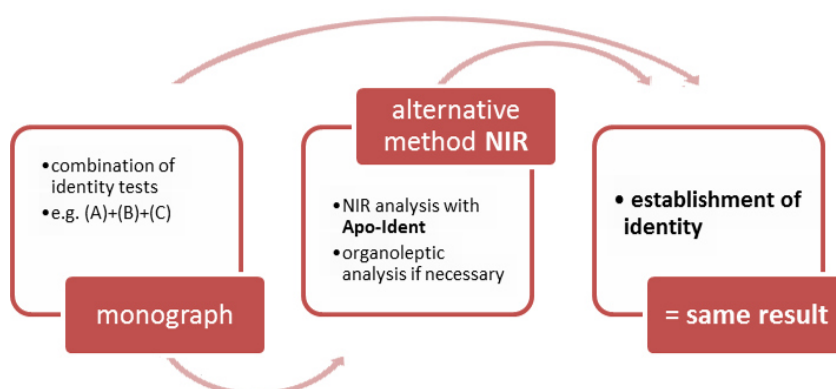


Figure 2: The combination of tests of the monograph is replaced by the alternative method NIR spectroscopy using *Apo-Ident*. This is permissible because both test procedures result in the establishment of the identity of the raw material.

With this validation documentation, proof is furnished that identical results are achieved with *Apo-Ident* and Pharmacopoeia methods, i.e. confirmation of the identity of the raw material [2].

Appendix E: Conformity of Apo-Ident with the European pharmacopeia

According to *Ph. Eur. Section 2.2.40*, NIR spectroscopy is basically suitable for: “Identification of agents, excipients, dosage forms, intermediate manufacturing products, chemical raw materials and packaging materials” ([3], quotation translated).

The fact that *Apo-Ident* meets the further criteria of the European Pharmacopoeia under the headings in *Section 2.2.40*

- Apparatus
- Measurement methods
- Sample preparation and presentation
- Testing the functionality of the instrument
- Identification and characterisation (qualitative analysis)
- Quantitative analysis
- Ongoing model evaluation
- Transfer of databases
- Data storage

can be proven based on the *HiperScan GmbH* documentation of “Meeting 2.2.40 *Ph. Eur.* by *Apo-Ident*” [4].

Appendix F: Addition to the second-stage models

As described in the general part of the *Apo-Ident* validation documentation, in the section [Model creation procedure and validation runs](#), under 2. *Generating the chemometric models (calibration)* in *f*), it is possible to create a further chemometric model for certain substances (second-stage model) and to undertake the assessment in several steps.

Substances in second-stage models

In the *Apo-Ident Update 2019-02*, a distinction is made between the following substances in the listed second-stage models:

Submodel 1

Bacitracin
Betamethasone, micronized
Betamethasone valerate
Budesonide, micronized
Capsaicin
Dexamethasone
Erythromycin
Heparin sodium
Hydrocortisone butyrate
Norethisterone acetate
Prednicarbate, micronized
Prednisolone, micronized
Prednisone
Triamcinolone, micronized
Triamcinolone acetonide

Submodel 2

Beclometasone dipropionate, anhydrous
Betamethasone dipropionate, micronized
Clobetasol propionate
Diphenylcyclopropenone
Gentamicin sulfate
Sodium benzoate
Sodium citrate
Oxybutynin hydrochloride

Submodel 3

Alfatradiol
Estriol
Pregnenolone
Progesterone, micronized
Quinine hydrochloride
Quinine sulfate dihydrate
Spironolactone
Testosterone propionate

Liquid submodel

2-ethylhexyl laurate
Base cream DAC

Lanette® ointment (conserved)
Non-ionic hydrophil ointment
Squalane
Wool alcohols cream DAB/SR

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