Validation documentation
TCM - Granulated herbal extracts (PhytoComm)

HiperScan GmbH

October 23, 2018

Validation documentation of the chemometrics database of the near-infrared spectrometer *Apo-Ident*.
Report number: **56-1.3-2018-07**
info@hiperscan.com, www.hiperscan.com

Contents

Introduction

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

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

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

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

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

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

Context of this document

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

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

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 *TCM - Granulated herbal extracts (PhytoComm)*. 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. Bezugsquellennachweis für Rezepturbestandteile* [Sources of supply for compounding] [7]).

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

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

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

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

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

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

2. Generating the chemometric models (calibration)

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

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

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

d) 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 *TCM - Granulated herbal extracts (PhytoComm)* 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 themself 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 14 000 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 Pharmacopeia* as a near-infrared spectrometer and proves the validity of the reference database with the existing validation documentation. This means that *Apo-Ident* can be used as an alternative testing method for testing raw materials at pharmacies.

Explanation of terminology

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

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

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

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

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

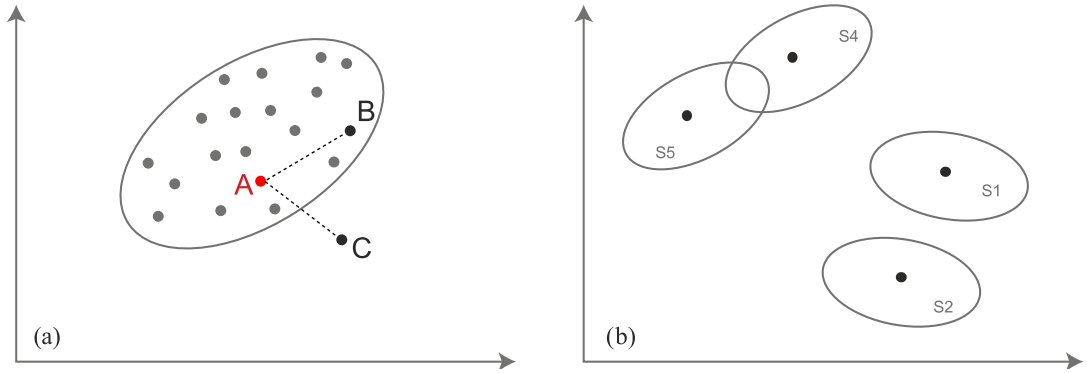

Figure 1: (a) The *Mahalanobis distance* from A to B is less than from A to C. However, the Euclidean distances are identical. (b) The *Mahalanobis distance* between the two measurement series *S4* and *S5* is smaller than between *S1* and *S2*. However, the Euclidean distances are identical.

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

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 23 740 spectra from 1131 different batches for a total of 268 substances were used to validate the substance class *TCM - Granulated herbal extracts (PhytoComm)*.

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
TCM - Granulated herbal extracts (PhytoComm)	141	178	14 240

From category *A* a total of 14 240 spectra from 178 batches for a total of 141 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
TCM - Granulated herbal extracts (PhytoComm)	144	181	7449

From category *B* a total of 7449 spectra from 181 batches for a total of 144 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
TCM - Granulated herbal extracts (PhytoComm)	268	975	2051

From category *C* a total of 2051 spectra from 975 batches for a total of 268 substances were taken into account for validation.

Validation results

The validation runs checked whether the substances/substance groups in the substance class *TCM - Granulated herbal extracts (PhytoComm)* can be distinguished from 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 *TCM - Granulated herbal extracts (PhytoComm)* 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	4	14 236	4	1 993 596
Type B	36	7173	36	1 043 064
Type C	377	213	1102	287 499

Some substances/substance groups in the substance class *TCM - Granulated herbal extracts (PhytoComm)* can only be distinguished from other substances with limitations. (*False positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	99.999 80 % (> 99.999 61 %)	99.971 70 % (> 99.945 67 %)
Type B	99.996 48 % (> 99.996 13 %)	99.493 48 % (> 99.441 60 %)
Type C	99.883 02 % (> 99.881 08 %)	12.715 87 % (> 12.372 15 %)

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

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

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ai Ye**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60407-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ai Ye; Artemisiae argyi folium

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ai Ye	G033H0613621	62017	40	from supplier
PhytoComm	Ai Ye	G033H0613621	62018	40	from supplier

Validation samples

A total of 23 740 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 *Ai Ye*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Ai Ye*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ai Ye	G033H0613621	62017†	20
PhytoComm	Ai Ye	G033H0613621	62018†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Ai Ye*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Ai Ye	G033H0613421	1
PhytoComm	Ai Ye	G033H0613021	2
Phytocomm	Ai Ye	G033H0613021	1
Phytocomm	Ai Ye	G033H0613022	1

- 2046 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ai Ye* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ai Ye* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	5	2046

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4534 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62017	62017	0.00	15.51
62018	62018	0.00	15.64

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ba Ji Tian**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60138-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ba Ji Tian; Morindae officinalis radix

Special notes

When selecting the *Ba Ji Tian* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ba Ji Tian	G165H0445621	61937	40	from supplier
PhytoComm	Ba Ji Tian	G165H0445621	61938	40	from supplier
PhytoComm	Ba Ji Tian	G165H0445621	62159	40	from supplier
PhytoComm	Ba Ji Tian	G165H0445621	62160	40	from supplier

Validation samples

A total of 23 740 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 *Ba Ji Tian*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Ba Ji Tian*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ba Ji Tian	G165H0445621	61937†	20
PhytoComm	Ba Ji Tian	G165H0445621	61938†	20
PhytoComm	Ba Ji Tian	G165H0445621	62159†	20
PhytoComm	Ba Ji Tian	G165H0445621	62160†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 6 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Ba Ji Tian*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Ba Ji Tian	G165H0445021	2
phytocomm	Ba Ji Tian	G165H0445021	2
PhytoComm	Ba Ji Tian	G165H0445222	1
PhytoComm	Ba Ji Tian	H0445921	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ba Ji Tian* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ba Ji Tian* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	12	0	6	2033

The substance/substance group *Ba Ji Tian* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	99.5526 % (> 99.2792 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61937	61937	0.00	8.32
61938	61938	0.00	8.50
62159	62159	0.00	7.09
62160	62160	0.00	7.02

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Bai Bian Dou**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60204-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bai Bian Dou; Dolichoris lablab semen

Special notes

When selecting the *Bai Bian Dou* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Bai Bian Dou	G093H0510522	62195	40	from supplier
PhytoComm	Bai Bian Dou	G093H0510522	62196	40	from supplier
PhytoComm	Bai Bian Dou	G093HS177QM1	62209	40	from supplier
PhytoComm	Bai Bian Dou	G093HS177QM1	62210	40	from supplier

Validation samples

A total of 23 740 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 *Bai Bian Dou*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Bai Bian Dou*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Bian Dou	G093H0510522	62195†	20
PhytoComm	Bai Bian Dou	G093H0510522	62196†	20
PhytoComm	Bai Bian Dou	G093HS177QM1	62209†	20
PhytoComm	Bai Bian Dou	G093HS177QM1	62210†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 3 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Bai Bian Dou*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Bai Bian Dou	G093H0510221	1
Phytocomm	Bai Bian Dou	g093h0510221	1
PhytoComm	Bai Bian Dou	H0510921	1

- 2048 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bai Bian Dou* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bai Bian Dou* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	8	0	3	2040

The substance/substance group *Bai Bian Dou* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	99.5558 % (> 99.2830 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62195	62195	0.00	19.50
62196	62196	0.00	19.64
62209	62209	0.00	12.19
62210	62210	0.00	11.27

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Bai He**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60093-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bai He; Lilii bulbus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Bai He	G139H0607622	62137	40	from supplier
PhytoComm	Bai He	G139H0607622	62138	40	from supplier

Validation samples

A total of 23 740 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 *Bai He*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Bai He*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai He	G139H0607622	62137†	20
PhytoComm	Bai He	G139H0607622	62138†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Bai He*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Bai He	G139H0607421	2
PhytoComm	Bai He	G139H0607421	1
Phytocomm	Bai He	g139h0607221	1
PhytoComm	Bai He	G139H0607221	1
PhytoComm	Bai He	G139H0607321	1
phytocomm	Bai He	H0607021	1
PhytoComm	Bai He	H0607021	2

- 2042 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bai He* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bai He* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	4	0	9	2038

The substance/substance group *Bai He* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.8342 % (> 99.5605 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62137	62137	0.00	11.81
62138	62138	0.00	11.92

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Bai Hua She She Cao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60039-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bai Hua She She Cao; Hedyotidis (diffusae) herba; Oldenlandiae diffusae herba

Special notes

When selecting the *Bai Hua She She Cao* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Bai Hua She She ...	G173H1153522	61967	40	from supplier
PhytoComm	Bai Hua She She ...	G173H1153522	61968	40	from supplier

Validation samples

A total of 23 740 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 *Bai Hua She She Cao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Bai Hua She She Cao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Hua She She Cao	G173H1153522	61967†	20
PhytoComm	Bai Hua She She Cao	G173H1153522	61968†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Bai Hua She She Cao*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Bai Hua She She Cao	G173H1153421	3
Phytocomm	Bai Hua She She Cao	G173H1153222	3
PhytoComm	Bai Hua She She Cao	G173H1153222	1
PhytoComm	Bai Hua She She Cao	H1153923	2

- 2042 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bai Hua She She Cao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bai Hua She She Cao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	9	2042

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4526 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61967	61967	0.00	20.24
61968	61968	0.00	20.58

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Bai Shao Yao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60007-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bai Shao Yao; Paeoniae lactiflorae albus radix

Special notes

When selecting the *Bai Shao Yao* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Bai Shao Yao	G179H0502521	61652	40	from supplier
PhytoComm	Bai Shao Yao	G179H0502522	61796	40	from supplier
PhytoComm	Bai Shao Yao	G179H0502522	61813	40	from supplier
PhytoComm	Bai Shao Yao	G179H0502621	61955	40	from supplier
PhytoComm	Bai Shao Yao	G179H0502621	61956	40	from supplier
PhytoComm	Bai Shao Yao	G179H0502721	62257	40	from supplier
PhytoComm	Bai Shao Yao	G179H0502721	62258	40	from supplier

Validation samples

A total of 23 740 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 *Bai Shao Yao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 4 different batches.

- 13 960 spectra from a total of 174 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 140 spectra from 7 reference samples of the substance/substance group *Bai Shao Yao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Shao Yao	G179H0502521	61652†	20
PhytoComm	Bai Shao Yao	G179H0502522	61796†	20
PhytoComm	Bai Shao Yao	G179H0502522	61813†	20
PhytoComm	Bai Shao Yao	G179H0502621	61955†	20
PhytoComm	Bai Shao Yao	G179H0502621	61956†	20
PhytoComm	Bai Shao Yao	G179H0502721	62257†	20
PhytoComm	Bai Shao Yao	G179H0502721	62258†	20

- 7309 spectra from a total of 177 batches from further 143 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 20 spectra from 11 *Apo-Ident* customers from 8 batches from the substance/substance group *Bai Shao Yao*.

- These include spectra of independent samples from 7 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Bai Shao Yao	G179H0502323	1
Phytocomm	Bai Shao Yao	G179H0502521	5
PhytoComm	Bai Shao Yao	1214401	1
PhytoComm	Bai Shao Yao	G179H0502025	1
Phytocomm	Bai Shao Yao	G179H0502025	3
PhytoComm	Bai Shao Yao	G179H0502121	1
Phytocomm	Bai Shao Yao	G179H0502121	2
PhytoComm	Bai Shao Yao	G179H0502322	2
Phytocomm	Bai Shao Yao	G179H0502322	1
Phytocomm	Bai Shao Yao	g179h0502322	1
Phytocomm	Bai Shao Yao	g17h0502323	1
phythocom	Bai Shao Yao	G179H0502121	1

- 2031 spectra from 17 *Apo-Ident* customers from a total of 966 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bai Shao Yao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bai Shao Yao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	13 960
Type B	0	140	0	7309
Type C	18	18	2	2013

The substance/substance group *Bai Shao Yao* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9477 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.8989 %)	100.0000 % (> 95.7143 %)
Type C	99.1831 % (> 98.9092 %)	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
61652	61652	0.00	13.57
61796	61796	0.00	15.53
61813	61813	0.00	13.32
61955	61955	0.00	8.84
61956	61956	0.00	8.81
62257	62257	0.00	6.03
62258	62258	0.00	6.00

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Bai Xian Pi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60208-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bai Xian Pi; Dictamni cortex; Dictamni dasycarpi cortex radicis

Special notes

When selecting the *Bai Xian Pi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Bai Xian Pi	G090H0515521	61707	40	from supplier
PhytoComm	Bai Xian Pi	G090HS355PM1	61849	40	from supplier
PhytoComm	Bai Xian Pi	G090HS355PM1	61850	40	from supplier

Validation samples

A total of 23 740 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 *Bai Xian Pi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 120 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 60 spectra from 3 reference samples of the substance/substance group *Bai Xian Pi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Xian Pi	G090H0515521	61707†	20
PhytoComm	Bai Xian Pi	G090HS355PM1	61849†	20
PhytoComm	Bai Xian Pi	G090HS355PM1	61850†	20

- 7389 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 7 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Bai Xian Pi*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Bai Xian Pi	G090H0515121	3
PhytoComm	Bai Xian Pi	G090H0515121	1
PhytoComm	Bai Xian Pi	H0515921	1
Phytocomm	Bai Xian Pi	H0515921	2

- 2044 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bai Xian Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bai Xian Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	1	14 120
Type B	0	47	13	7389
Type C	4	0	7	2040

The substance/substance group *Bai Xian Pi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	99.1667 % (> 96.6667 %)
Type B	100.0000 % (> 99.8992 %)	78.3333 % (> 73.3333 %)
Type C	99.8342 % (> 99.5606 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61707	61707	0.00	8.76
61849	61849	0.00	4.19
61850	61850	0.00	4.20

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Bai Zhu**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60015-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bai Zhu; Atractylodis macrocephalae rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Bai Zhu	G041H0501621	61837	40	from supplier
PhytoComm	Bai Zhu	G041H0501721	62219	40	from supplier
PhytoComm	Bai Zhu	G041H0501721	62220	40	from supplier

Validation samples

A total of 23 740 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 *Bai Zhu*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 120 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 60 spectra from 3 reference samples of the substance/substance group *Bai Zhu*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Zhu	G041H0501621	61837†	20
PhytoComm	Bai Zhu	G041H0501721	62219†	20
PhytoComm	Bai Zhu	G041H0501721	62220†	20

- 7389 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 21 spectra from 9 *Apo-Ident* customers from 5 batches from the substance/substance group *Bai Zhu*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phythocom	Bai Zhu	G041H0501221	4
phythocom	Bai Zhu	g041h0501221	2
phythocom	Bai Zhu	h0501021	1
Phytocomm	Bai Zhu	G041H0501422	2
PhytoComm	Bai Zhu	G041H0501221	1
Phytocomm	Bai Zhu	G041H0501221	3
Phytocomm	Bai Zhu	g041h0501221	3
PhytoComm	Bai Zhu	H0501021	1
Phytocomm	Bai Zhu	H0501021	4

- 2030 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bai Zhu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bai Zhu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 120
Type B	1	60	0	7388
Type C	1	0	21	2029

The substance/substance group *Bai Zhu* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 95.0000 %)
Type B	99.9913 % (> 99.9409 %)	100.0000 % (> 90.0000 %)
Type C	99.9751 % (> 99.7012 %)	0.0000 % (≥ 0.0000 %)

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
61837	61837	0.00	11.80
62219	62219	0.00	6.09
62220	62220	0.00	6.90

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Bai Zi Ren**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60197-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bai Zi Ren; Biotae orientalis semen; Platycladi semen

Special notes

When selecting the *Bai Zi Ren* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Bai Zi Ren	`G052HS187PG1`	`61848`	40	from supplier

Validation samples

A total of 23 740 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 *Bai Zi Ren*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Bai Zi Ren*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Zi Ren	G052HS187PG1	61848†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 batches from the substance/substance group *Bai Zi Ren*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Bai Zi Ren	g052f110315	1
Phytocomm	Bai Zi Ren	G052HS187	2
Phytocomm	Bai Zi Ren	g952f110315	1
phythocom	Bai Zi Ren	G052F110315	1

- 2046 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bai Zi Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bai Zi Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	0	0	5	2046

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.4534 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61848	61848	0.00	10.58

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ban Lan Gen**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60230-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ban Lan Gen; Isatidis radix

Special notes

When selecting the *Ban Lan Gen* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ban Lan Gen	G128H0816521	61993	40	from supplier
PhytoComm	Ban Lan Gen	G128H0816521	61994	40	from supplier

Validation samples

A total of 23 740 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 *Ban Lan Gen*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Ban Lan Gen*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ban Lan Gen	G128H0816521	61993†	20
PhytoComm	Ban Lan Gen	G128H0816521	61994†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Ban Lan Gen*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Ban Lan Gen	G128H0816421	2
PhytoComm	Ban Lan Gen	G128H0816022	1
Phytocomm	Ban Lan Gen	G128H0816022	2
Phytocomm	Ban Lan Gen	G128H0816221	3
PhytoComm	Ban Lan Gen	G128H0816221	2
Herbasinica	Ban Lan Gen	GENTIANAEMACROPHYLL	1
PhytoComm	Ban Lan Gen	H0816922	1

- 2039 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ban Lan Gen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ban Lan Gen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	9	3	9	2030

The substance/substance group *Ban Lan Gen* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.6765 % (> 99.4027 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61993	61993	0.00	9.29
61994	61994	0.00	8.54

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ban Xia (Jiang)**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60019-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ban Xia (Jiang); Pinelliae rhizoma praeparatum cum zingibere

Special notes

When selecting the *Ban Xia (Jiang)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ban Xia (Jiang)	G191H0526521	61786	40	from supplier
PhytoComm	Ban Xia (Jiang)	G191H0526521	61829	40	from supplier
PhytoComm	Ban Xia (Jiang)	G191HS090QL1	62201	40	from supplier
PhytoComm	Ban Xia (Jiang)	G191HS090QL1	62202	40	from supplier

Validation samples

A total of 23 740 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 *Ban Xia (Jiang)*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Ban Xia (Jiang)*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ban Xia (Jiang)	G191H0526521	61786†	20
PhytoComm	Ban Xia (Jiang)	G191H0526521	61829†	20
PhytoComm	Ban Xia (Jiang)	G191HS090QL1	62201†	20
PhytoComm	Ban Xia (Jiang)	G191HS090QL1	62202†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 11 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Ban Xia (Jiang)*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Ban Xia (Jiang)	G191H0526023	1
PhytoComm	Ban Xia (Jiang)	G191H0526023	1
Phytocomm	Ban Xia (Jiang)	G191H0526121	6
PhytoComm	Ban Xia (Jiang)	G191H0526121	1
Phytocomm	Ban Xia (Jiang)	g191h0526121	1
Phytocomm	Ban Xia (Jiang)	G191H0526322	1

- 2040 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	3	160	0	14 077
Type B	9	80	0	7360
Type C	0	0	11	2040

The substance/substance group *Ban Xia (Jiang)* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	99.9776 % (> 99.9515 %)	100.0000 % (> 96.2500 %)
Type B	99.8413 % (> 99.7908 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61786	61786	0.00	29.38
61829	61829	0.00	30.06
62201	62201	0.00	4.53
62202	62202	0.00	5.40

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ban Zhi Lian**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60038-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ban Zhi Lian; Scutellariae barbatae herba

Special notes

When selecting the *Ban Zhi Lian* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ban Zhi Lian	G224H0528521	61362	40	from supplier
PhytoComm	Ban Zhi Lian	G224H0528522	61921	40	from supplier
PhytoComm	Ban Zhi Lian	G224H0528522	61922	40	from supplier

Validation samples

A total of 23 740 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 *Ban Zhi Lian*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 120 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 60 spectra from 3 reference samples of the substance/substance group *Ban Zhi Lian*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ban Zhi Lian	G224H0528521	61362†	20
PhytoComm	Ban Zhi Lian	G224H0528522	61921†	20
PhytoComm	Ban Zhi Lian	G224H0528522	61922†	20

- 7389 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 6 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Ban Zhi Lian*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Ban Zhi Lian	G224H0528521	2
PhytoComm	Ban Zhi Lian	G224H0528521	1
Herbasin	Ban Zhi Lian	G224H0528022	1
Phytocomm	Ban Zhi Lian	G224H0528221	1
PhytoComm	Ban Zhi Lian	H0528021	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ban Zhi Lian* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ban Zhi Lian* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 120
Type B	0	60	0	7389
Type C	0	3	3	2045

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.8992 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.4531 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61362	61362	0.00	16.55
61921	61921	0.00	9.13
61922	61922	0.00	9.64

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Bu Gu Zhi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60023-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bu Gu Zhi; Psoraleae corylifoliae fructus

Special notes

When selecting the *Bu Gu Zhi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Bu Gu Zhi	G205H1247621	61939	40	from supplier
PhytoComm	Bu Gu Zhi	G205H1247621	61940	40	from supplier

Validation samples

A total of 23 740 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 *Bu Gu Zhi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Bu Gu Zhi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bu Gu Zhi	G205H1247621	61939†	20
PhytoComm	Bu Gu Zhi	G205H1247621	61940†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Bu Gu Zhi*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Bu Gu Zhi	G205H1247421	2
Phytocomm	Bu Gu Zhi	G205H1247222	2
Phytocomm	Bu Gu Zhi	g205h1247222	1
PhytoComm	Bu Gu Zhi	H1247021	4

- 2042 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bu Gu Zhi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bu Gu Zhi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	1	8	2041

The substance/substance group *Bu Gu Zhi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9751 % (> 99.7014 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61939	61939	0.00	10.26
61940	61940	0.00	10.45

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Cang Er Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60054-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cang Er Zi; Xanthii fructus

Special notes

When selecting the *Cang Er Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Cang Er Zi	G251H1401622	61897	40	from supplier
PhytoComm	Cang Er Zi	G251H1401622	61898	40	from supplier
PhytoComm	Cang Er Zi	G251H1401622	62155	40	from supplier
PhytoComm	Cang Er Zi	G251H1401622	62156	40	from supplier

Validation samples

A total of 23 740 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 *Cang Er Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Cang Er Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Cang Er Zi	G251H1401622	61897†	20
PhytoComm	Cang Er Zi	G251H1401622	61898†	20
PhytoComm	Cang Er Zi	G251H1401622	62155†	20
PhytoComm	Cang Er Zi	G251H1401622	62156†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 15 spectra from 8 *Apo-Ident* customers from 7 batches from the substance/substance group *Cang Er Zi*.

- These include spectra of independent samples from 7 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Cang Er Zi	G251H1401021	2
PhytoComm	Cang Er Zi	(251)H1401021	1
PhytoComm	Cang Er Zi	G251H1401021	1
Phytocomm	Cang Er Zi	g251h1401021	1
Phytocomm	Cang Er Zi	G251H1401123	4
Phytocomm	Cang Er Zi	G251H1401322	2
PhytoComm	Cang Er Zi	G251H1401322	1
Phytocomm	Cang Er Zi	G251H1401521	1
Phytocomm	Cang Er Zi	H1401021	1
PhytoComm	Cang Er Zi	H1401021	1

- 2036 spectra from 17 *Apo-Ident* customers from a total of 967 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cang Er Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cang Er Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	0	9	6	2036

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4523 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61897	61897	0.00	17.46
61898	61898	0.00	18.22
62155	62155	0.00	23.89
62156	62156	0.00	23.88

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Cang Zhu**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60160-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cang Zhu; Atractylodis rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Cang Zhu	G042H1402521	61767	40	from supplier
PhytoComm	Cang Zhu	G042H1402521	61800	40	from supplier

Validation samples

A total of 23 740 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 *Cang Zhu*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Cang Zhu*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Cang Zhu	G042H1402521	61767†	20
PhytoComm	Cang Zhu	G042H1402521	61800†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 8 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Cang Zhu*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Cang Zhu	G042H1402221	2
PhytoComm	Cang Zhu	G042H1402221	1
Phytocomm	Cang Zhu	g042h1402221	1
PhytoComm	Cang Zhu	G042H1402321	1
PhytoComm	Cang Zhu	H1402922	1
Phytocomm	Cang Zhu	H1402922	2

- 2043 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cang Zhu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cang Zhu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	4	0	8	2039

The substance/substance group *Cang Zhu* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.8321 % (> 99.5585 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61767	61767	0.00	4.78
61800	61800	0.00	4.91

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Chai Hu**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60010-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chai Hu; Bupleuri radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Chai Hu	G055H1055721	62099	40	from supplier
PhytoComm	Chai Hu	G055H1055721	62100	40	from supplier

Validation samples

A total of 23 740 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 *Chai Hu*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Chai Hu*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chai Hu	G055H1055721	62099†	20
PhytoComm	Chai Hu	G055H1055721	62100†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 16 spectra from 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Chai Hu*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Chai Hu	G055H1055422	5
PhytoComm	Chai Hu	G044H1055322	1
PhytoComm	Chai Hu	G055H1055123	1
Phytocomm	Chai Hu	G055H1055123	5
Phytocomm	Chai Hu	g055h1055123	1
PhytoComm	Chai Hu	G055H1055322	1
PhytoComm	Chai Hu	H1055022	1
Phytocomm	Chai Hu	H1055022	1

- 2035 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chai Hu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chai Hu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	18	1	15	2017

The substance/substance group *Chai Hu* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.2515 % (> 98.9777 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62099	62099	0.00	9.48
62100	62100	0.00	9.44

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Che Qian Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60255-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Che Qian Zi; Plantaginis semen

Special notes

When selecting the *Che Qian Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Che Qian Zi	G192H0723621	61963	40	from supplier
PhytoComm	Che Qian Zi	G192H0723621	61964	40	from supplier

Validation samples

A total of 23 740 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 *Che Qian Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Che Qian Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Che Qian Zi	G192H0723621	61963†	20
PhytoComm	Che Qian Zi	G192H0723621	61964†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 8 *Apo-Ident* customers from 4 batches from the substance/substance group *Che Qian Zi*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Che Qian Zi	G192H0723321	3
PhytoComm	Che Qian Zi	410704805	1
Phytocomm	Che Qian Zi	G192H0723421	2
Phytocomm	Che Qian Zi	410704805	1
PhytoComm	Che Qian Zi	G192H0723121	1
Phytocomm	Che Qian Zi	G192H0723121	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Che Qian Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Che Qian Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	9	2042

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4526 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61963	61963	0.00	68.22
61964	61964	0.00	70.19

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Chen Pi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60009-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chen Pi; Citri reticulatae pericarpium

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Chen Pi	G073H1128621	61841	40	from supplier

Validation samples

A total of 23 740 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 *Chen Pi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Chen Pi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chen Pi	G073H1128621	61841†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Chen Pi*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Chen Pi	G073H1128221	1
Phytocomm	Chen Pi	G073H1128222	2
PhytoComm	Chen Pi	G073H1128221	1
PhytoComm	Chen Pi	G073H1128222	2
Phytocomm	Chen Pi	g073h1128222	1
Phytocomm	Chen Pi	g07h1128221	1
PhytoComm	Chen Pi	H1128922	1
phythocom	Chen Pi	g073h1128221	1

- 2041 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chen Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chen Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	4	0	10	2037

The substance/substance group *Chen Pi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	99.8559 % (> 99.5822 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61841	61841	0.00	9.01

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Chuan Lian Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60078-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chuan Lian Zi; Meliae toosendan fructus

Special notes

When selecting the *Chuan Lian Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Chuan Lian Zi	G157H0306621	62127	40	from supplier
PhytoComm	Chuan Lian Zi	G157H0306621	62128	40	from supplier
PhytoComm	Chuan Lian Zi	G157H0306621	62177	40	from supplier
PhytoComm	Chuan Lian Zi	G157H0306621	62178	40	from supplier

Validation samples

A total of 23 740 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 *Chuan Lian Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Chuan Lian Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chuan Lian Zi	G157H0306621	62127†	20
PhytoComm	Chuan Lian Zi	G157H0306621	62128†	20
PhytoComm	Chuan Lian Zi	G157H0306621	62177†	20
PhytoComm	Chuan Lian Zi	G157H0306621	62178†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 9 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Chuan Lian Zi*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Chuan Lian Zi	G157H0306421	2
Phytocomm	Chuan Lian Zi	G157H0306421	1
PhytoComm	Chuan Lian Zi	G157H0305221	1
Phytocomm	Chuan Lian Zi	G157H0306121	1
PhytoComm	Chuan Lian Zi	G157H0306121	3
Phytocomm	Chuan Lian Zi	H0306921	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chuan Lian Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chuan Lian Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 080
Type B	0	79	1	7369
Type C	5	3	6	2037

The substance/substance group *Chuan Lian Zi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	98.7500 % (> 95.0000 %)
Type C	99.8134 % (> 99.5398 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62127	62127	0.00	6.13
62128	62128	0.00	5.68
62177	62177	0.00	6.87
62178	62178	0.00	6.31

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Chuan Niu Xi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60122-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chuan Niu Xi; Cyathulae radix

Special notes

When selecting the *Chuan Niu Xi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Chuan Niu Xi	G318H0431621	61883	40	from supplier
PhytoComm	Chuan Niu Xi	G318H0431621	61884	40	from supplier

Validation samples

A total of 23 740 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 *Chuan Niu Xi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Chuan Niu Xi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chuan Niu Xi	G318H0431621	61883†	20
PhytoComm	Chuan Niu Xi	G318H0431621	61884†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Chuan Niu Xi*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Chuan Niu Xi	g318h0431321	1
PhytoComm	Chuan Niu Xi	G318H0431321	1
PhytoComm	Chuan Niu Xi	H0431923	3

- 2046 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chuan Niu Xi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chuan Niu Xi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	0	5	2045

The substance/substance group *Chuan Niu Xi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9378 % (> 99.6645 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61883	61883	0.00	6.62
61884	61884	0.00	5.84

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Chuan Xiong**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60013-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chuan Xiong; Ligustici chuanxiong rhizoma; Ligustici wallichii radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Chuan Xiong	G136H0305621	61975	40	from supplier
PhytoComm	Chuan Xiong	G136H0305621	61976	40	from supplier

Validation samples

A total of 23 740 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 *Chuan Xiong*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Chuan Xiong*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chuan Xiong	G136H0305621	61975†	20
PhytoComm	Chuan Xiong	G136H0305621	61976†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Chuan Xiong*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Chuan Xiong	G136H0305421	1
Phytocomm	Chuan Xiong	G135H0305121	1
phytocomm	Chuan Xiong	G136H0305121	1
PhytoComm	Chuan Xiong	G136H0305121	1
Phytocomm	Chuan Xiong	G136H0305121	3
Phytocomm	Chuan Xiong	g136h0305121	1
PhytoComm	Chuan Xiong	G136H0305221	2
Phytocomm	Chuan Xiong	G136H0305221	1
Phytocomm	Chuan Xiong	G136H305121	1

- 2039 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chuan Xiong* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chuan Xiong* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	0	12	2038

The substance/substance group *Chuan Xiong* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9534 % (> 99.6796 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61975	61975	0.00	6.97
61976	61976	0.00	6.97

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ci Wu Jia**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60354-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ci Wu Jia; Acanthopanacis (senticosi) radix; Eleutherococci radix

Special notes

When selecting the *Ci Wu Jia* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ci Wu Jia	`G302H0856621`	`62117`	40	from supplier
PhytoComm	Ci Wu Jia	`G302H0856621`	`62118`	40	from supplier

Validation samples

A total of 23 740 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 *Ci Wu Jia*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Ci Wu Jia*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ci Wu Jia	G302H0856621	62117†	20
PhytoComm	Ci Wu Jia	G302H0856621	62118†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 *Ci Wu Jia*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Ci Wu Jia	G302H0856022	1
Phytocomm	Ci Wu Jia	G302H0856121	1

- 2049 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ci Wu Jia* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ci Wu Jia* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	5	0	2	2044

The substance/substance group *Ci Wu Jia* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.7916 % (> 99.5196 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62117	62117	0.00	10.55
62118	62118	0.00	10.64

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Da Huang**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60140-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Da Huang; Rhei radix et rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Da Huang	G212H0320622	62129	40	from supplier
PhytoComm	Da Huang	G212H0320622	62130	40	from supplier
PhytoComm	Da Huang	G212H0320622	62157	40	from supplier
PhytoComm	Da Huang	G212H0320622	62158	40	from supplier

Validation samples

A total of 23 740 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 *Da Huang*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Da Huang*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Da Huang	G212H0320622	62129†	20
PhytoComm	Da Huang	G212H0320622	62130†	20
PhytoComm	Da Huang	G212H0320622	62157†	20
PhytoComm	Da Huang	G212H0320622	62158†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 10 spectra from 7 *Apo-Ident* customers from 4 batches from the substance/substance group *Da Huang*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Da Huang	G212H0320521	3
PhytoComm	Da Huang	G212H0320023	1
Phytocomm	Da Huang	G212H0320023	1
Phytocomm	Da Huang	g212h0320023	1
PhytoComm	Da Huang	G212H0320321	2
Phytocomm	Da Huang	G212H0320321	2

- 2041 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Da Huang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Da Huang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	0	6	4	2041

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62129	62129	0.00	108.10
62130	62130	0.00	107.76
62157	62157	0.00	91.73
62158	62158	0.00	92.50

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Da Qing Ye**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60256-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Da Qing Ye; Isatidis folium

Special notes

When selecting the *Da Qing Ye* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Da Qing Ye	G127H0318621	62003	40	from supplier
PhytoComm	Da Qing Ye	G127H0318621	62004	40	from supplier
PhytoComm	Da Qing Ye	G127H0318621	62161	40	from supplier
PhytoComm	Da Qing Ye	G127H0318621	62162	40	from supplier

Validation samples

A total of 23 740 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 *Da Qing Ye*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Da Qing Ye*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Da Qing Ye	G127H0318621	62003†	20
PhytoComm	Da Qing Ye	G127H0318621	62004†	20
PhytoComm	Da Qing Ye	G127H0318621	62161†	20
PhytoComm	Da Qing Ye	G127H0318621	62162†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 7 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Da Qing Ye*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Da Qing Ye	4103167001	1
phytocomm	Da Qing Ye	410316901	1
Phytocomm	Da Qing Ye	G127H0318121	1
Herbasin	Da Qing Ye	G127H0318121	1
PhytoComm	Da Qing Ye	G127H0318121	1
Phytocomm	Da Qing Ye	G127H0318421	2

- 2044 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Da Qing Ye* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Da Qing Ye* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	0	5	2	2044

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4529 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62003	62003	0.00	18.52
62004	62004	0.00	17.78
62161	62161	0.00	13.55
62162	62162	0.00	13.98

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Da Zao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60055-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Da Zao; Zizyphi jujubae fructus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Da Zao	G129H0316521	61730	40	from supplier
PhytoComm	Da Zao	G129H0316621	62215	40	from supplier
PhytoComm	Da Zao	G129H0316621	62216	40	from supplier

Validation samples

A total of 23 740 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 *Da Zao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 120 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 60 spectra from 3 reference samples of the substance/substance group *Da Zao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Da Zao	G129H0316521	61730†	20
PhytoComm	Da Zao	G129H0316621	62215†	20
PhytoComm	Da Zao	G129H0316621	62216†	20

- 7389 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 16 spectra from 7 *Apo-Ident* customers from 4 batches from the substance/substance group *Da Zao*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Da Zao	G129H0316521	3
phytocomm	Da Zao	G129H0316121	2
PhytoComm	Da Zao	G129H0316121	1
Phytocomm	Da Zao	G129H0316121	5
PhytoComm	Da Zao	G129H0316221	1
Phytocomm	Da Zao	G129H0316221	3
Phytocomm	Da Zao	g129h0316221	1

- 2035 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Da Zao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Da Zao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 120
Type B	0	60	0	7389
Type C	3	7	9	2032

The substance/substance group *Da Zao* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.8992 %)	100.0000 % (> 90.0000 %)
Type C	99.8756 % (> 99.6017 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61730	61730	0.00	10.97
62215	62215	0.00	16.57
62216	62216	0.00	15.68

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Dan Dou Chi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60794-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dan Dou Chi; Sojae semen praeparatum

Special notes

When selecting the *Dan Dou Chi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Dan Dou Chi	G232H1106621	61909	40	from supplier
PhytoComm	Dan Dou Chi	G232H1106621	61910	40	from supplier
PhytoComm	Dan Dou Chi	G232H1106621	62173	40	from supplier
PhytoComm	Dan Dou Chi	G232H1106621	62174	40	from supplier

Validation samples

A total of 23 740 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 *Dan Dou Chi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 75 spectra from 4 reference samples of the substance/substance group *Dan Dou Chi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dan Dou Chi	G232H1106621	61909†	20
PhytoComm	Dan Dou Chi	G232H1106621	61910†	20
PhytoComm	Dan Dou Chi	G232H1106621	62173†	20
PhytoComm	Dan Dou Chi	G232H1106621	62174†	15

- 7374 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Dan Dou Chi*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Dan Dou Chi	G232HS239	1
PhytoComm	Dan Dou Chi	G232H1106321	1

- 2049 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dan Dou Chi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dan Dou Chi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 080
Type B	0	75	0	7374
Type C	0	0	2	2049

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8991 %)	100.0000 % (> 92.0000 %)
Type C	100.0000 % (> 99.4559 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61909	61909	0.00	45.84
61910	61910	0.00	46.61
62173	62173	0.00	68.57
62174	62174	0.00	68.71

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Dan Shen**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60030-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dan Shen; Salviae miltiorrhizae radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Dan Shen	G214H0441422	61367	40	from supplier
PhytoComm	Dan Shen	G214H0441522	61731	40	from supplier
PhytoComm	Dan Shen	G214H0441522	62063	40	from supplier
PhytoComm	Dan Shen	G214H0441522	62064	40	from supplier

Validation samples

A total of 23 740 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 *Dan Shen*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Dan Shen*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dan Shen	G214H0441422	61367†	20
PhytoComm	Dan Shen	G214H0441522	61731†	20
PhytoComm	Dan Shen	G214H0441522	62063†	20
PhytoComm	Dan Shen	G214H0441522	62064†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 16 spectra from 8 *Apo-Ident* customers from 5 batches from the substance/substance group *Dan Shen*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Dan Shen	G214H0441522	1
PhytoComm	Dan Shen	G214H0441522	1
Phytocomm	Dan Shen	G214H0441121	5
PhytoComm	Dan Shen	G214H0441121	2
Phytocomm	Dan Shen	g214h0441121	1
PhytoComm	Dan Shen	G214H0441221	2
Phytocomm	Dan Shen	G214H0441221	1
Phytocomm	Dan Shen	G214H0441322	1
PhytoComm	Dan Shen	G214H0441322	2

- 2035 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dan Shen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dan Shen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 080
Type B	0	80	0	7369
Type C	2	12	4	2033

The substance/substance group *Dan Shen* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	99.9005 % (> 99.6266 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61367	61367	0.00	10.40
61731	61731	0.00	11.78
62063	62063	0.00	8.97
62064	62064	0.00	8.96

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Dan Zhu Ye**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60147-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dan Zhu Ye; Lophatheri gracilis herba

Special notes

When selecting the *Dan Zhu Ye* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Dan Zhu Ye	`G046H1105621`	`62105`	40	from supplier
PhytoComm	Dan Zhu Ye	`G046H1105621`	`62106`	40	from supplier

Validation samples

A total of 23 740 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 *Dan Zhu Ye*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Dan Zhu Ye*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dan Zhu Ye	G046H1105621	62105†	20
PhytoComm	Dan Zhu Ye	G046H1105621	62106†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Dan Zhu Ye*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Dan Zhu Ye	G046H1105021	2
PhytoComm	Dan Zhu Ye	G046H1105021	1
Phytocomm	Dan Zhu Ye	G046H1105321	4
Phytocomm	Dan Zhu Ye	G046H110521	1
PhytoComm	Dan Zhu Ye	H1105921	2

- 2041 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dan Zhu Ye* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dan Zhu Ye* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	11	0	10	2030

The substance/substance group *Dan Zhu Ye* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.2354 % (> 98.9616 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62105	62105	0.00	7.67
62106	62106	0.00	8.15

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Dang Gui**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60003-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dang Gui; Angelicae sinensis radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Dang Gui	G022H1306721	62223	40	from supplier
PhytoComm	Dang Gui	G022H1306721	62224	40	from supplier

Validation samples

A total of 23 740 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 *Dang Gui*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Dang Gui*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dang Gui	G022H1306721	62223†	20
PhytoComm	Dang Gui	G022H1306721	62224†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 19 spectra from 9 *Apo-Ident* customers from 8 batches from the substance/substance group *Dang Gui*.

- These include spectra of independent samples from 8 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Dang Gui	G022H1306422	2
PhytoComm	Dang Gui	G022H1306621	2
PhytoComm	Dang Gui	G022H1306022	2
Phytocomm	Dang Gui	G022H1306022	5
Phytocomm	Dang Gui	G022H1306023	1
Phytocomm	Dang Gui	G022H1306121	1
Phytocomm	Dang Gui	g022h1306121	3
PhytoComm	Dang Gui	G022H1306121	1
PhytoComm	Dang Gui	G022H1306321	1
PhytoComm	Dang Gui	G13-0784	1

- 2032 spectra from 17 *Apo-Ident* customers from a total of 966 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dang Gui* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dang Gui* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	23	5	14	2009

The substance/substance group *Dang Gui* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.2465 % (> 98.9726 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62223	62223	0.00	7.60
62224	62224	0.00	7.02

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Dang Gui Wei**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60308-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dang Gui Wei; Angelicae sinensis radix extremitas

Special notes

When selecting the *Dang Gui Wei* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Dang Gui Wei	G312H1307621	61885	40	from supplier
PhytoComm	Dang Gui Wei	G312H1307621	61886	40	from supplier

Validation samples

A total of 23 740 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 *Dang Gui Wei*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Dang Gui Wei*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dang Gui Wei	G312H1307621	61885†	20
PhytoComm	Dang Gui Wei	G312H1307621	61886†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 8 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Dang Gui Wei*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Dang Gui Wei	(G312)H1307021	1
PhytoComm	Dang Gui Wei	G312H1307021	2
Phytocomm	Dang Gui Wei	G312H1307021	5

- 2043 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dang Gui Wei* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dang Gui Wei* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	7	0	8	2036

The substance/substance group *Dang Gui Wei* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.7775 % (> 99.5038 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61885	61885	0.00	11.93
61886	61886	0.00	12.02

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Di Gu Pi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60036-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Di Gu Pi; Lycii chinensis radicis cortex

Special notes

When selecting the *Di Gu Pi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Di Gu Pi	G149H0601622	62211	40	from supplier
PhytoComm	Di Gu Pi	G149H0601622	62212	40	from supplier

Validation samples

A total of 23 740 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 *Di Gu Pi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Di Gu Pi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Di Gu Pi	G149H0601622	62211†	20
PhytoComm	Di Gu Pi	G149H0601622	62212†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Di Gu Pi*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Di Gu Pi	G149H0601421	1
PhytoComm	Di Gu Pi	G149H0601421	2
Phytocomm	Di Gu Pi	g149h060112	1
PhytoComm	Di Gu Pi	G149H0601122	2
Phytocomm	Di Gu Pi	G149H0601122	1
Phytocomm	Di Gu Pi	G149H0601822	1
PhytoComm	Di Gu Pi	H0601821	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Di Gu Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Di Gu Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	4	0	9	2038

The substance/substance group *Di Gu Pi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.8673 % (> 99.5936 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62211	62211	0.00	9.69
62212	62212	0.00	10.17

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Dong Gua Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60202-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dong Gua Zi; Benincasae hispidae semen

Special notes

When selecting the *Dong Gua Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Dong Gua Zi	G049H0551622	62015	40	from supplier
PhytoComm	Dong Gua Zi	G049H0551622	62016	40	from supplier

Validation samples

A total of 23 740 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 *Dong Gua Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Dong Gua Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dong Gua Zi	G049H0551622	62015†	20
PhytoComm	Dong Gua Zi	G049H0551622	62016†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 7 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Dong Gua Zi*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Dong Gua Zi	G049H0551221	5
Phytocomm	Dong Gua Zi	G049H0551021	1
PhytoComm	Dong Gua Zi	G049H0551221	1

- 2044 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dong Gua Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dong Gua Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	7	2044

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4529 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62015	62015	0.00	31.71
62016	62016	0.00	31.67

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Dong Kui Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60483-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dong Kui Zi; Abutili semen; Malvae semen

Special notes

When selecting the *Dong Kui Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Dong Kui Zi	G001H0834721	62089	40	from supplier
PhytoComm	Dong Kui Zi	G001H0834721	62090	40	from supplier

Validation samples

A total of 23 740 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 *Dong Kui Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Dong Kui Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dong Kui Zi	G001H0834721	62089†	20
PhytoComm	Dong Kui Zi	G001H0834721	62090†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 *Dong Kui Zi*.

- These include spectra of independent samples from 1 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Dong Kui Zi	G001BP030505	1

- 2050 spectra from 17 *Apo-Ident* customers from a total of 973 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dong Kui Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dong Kui Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	1	2050

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4601 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62089	62089	0.00	28.60
62090	62090	0.00	28.14

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**E Zhu**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`50344-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

E Zhu; Curcumae zedoariae rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	E Zhu	`G083H1110521`	`61741`	40	from supplier

Validation samples

A total of 23 740 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 *E Zhu*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *E Zhu*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	E Zhu	G083H1110521	61741†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 5 *Apo-Ident* customers from 5 batches from the substance/substance group *E Zhu*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	E Zhu	(083)H1110021	1
Phytocomm	E Zhu	G083H111022	1
PhytoComm	E Zhu	G083H1110222	3
PhytoComm	E Zhu	H1110021	2
Phytocomm	E Zhu	H1110021	2
Phytocomm	E Zhu	h1110021	1

- 2041 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *E Zhu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *E Zhu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	2	0	10	2039

The substance/substance group *E Zhu* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	99.9194 % (> 99.6457 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61741	61741	0.00	10.58

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Fang Feng**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`50261-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fang Feng; Saposhnikoviae radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Fang Feng	`G217H0728621`	`62237`	40	from supplier
PhytoComm	Fang Feng	`G217H0728621`	`62238`	40	from supplier

Validation samples

A total of 23 740 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 *Fang Feng*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Fang Feng*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fang Feng	G217H0728621	62237†	20
PhytoComm	Fang Feng	G217H0728621	62238†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 19 spectra from 9 *Apo-Ident* customers from 8 batches from the substance/substance group *Fang Feng*.

- These include spectra of independent samples from 8 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Fang Feng	G217H0728521	3
PhytoComm	Fang Feng	G217H0728521	2
Phytocomm	Fang Feng	G217H0728221	1
Phytocomm	Fang Feng	g217h0728221	1
PhytoComm	Fang Feng	G217H0728221	1
Phytocomm	Fang Feng	G217H0728923	4
PhytoComm	Fang Feng	G217H0728923	1
Phytocomm	Fang Feng	g217h0728923	1
Phytocomm	Fang Feng	G217H728923	1
Phytocomm	Fang Feng	G21H0728923	1
phytocomm	Fang Feng	H0728922	1
Phytocomm	Fang Feng	H0728922	1
phythocom	Fang Feng	G217H0728923	1

- 2032 spectra from 17 *Apo-Ident* customers from a total of 966 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fang Feng* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fang Feng* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	22	4	15	2010

The substance/substance group *Fang Feng* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.4670 % (> 99.1930 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62237	62237	0.00	11.02
62238	62238	0.00	11.14

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Fang Ji**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60270-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fang Ji; Stephaniae tetrandrae radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Fang Ji	G236HS122QM1	62179	40	from supplier
PhytoComm	Fang Ji	G236HS122QM1	62180	40	from supplier

Validation samples

A total of 23 740 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 *Fang Ji*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Fang Ji*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fang Ji	G236HS122QM1	62179†	20
PhytoComm	Fang Ji	G236HS122QM1	62180†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 3 batches from the substance/substance group *Fang Ji*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Herbasin	Fang Ji	G236H0727123	1
PhytoComm	Fang Ji	G236H0727123	1
Phytocomm	Fang Ji	G236H0727321	2
phytocomm	Fang Ji	FA0727901	1
Phytocomm	Fang Ji	FA0727901	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fang Ji* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fang Ji* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	6	2045

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4531 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62179	62179	0.00	17.85
62180	62180	0.00	18.13

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Fo Shou**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60119-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fo Shou; Citri sarcodactylis fructus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Fo Shou	`G307HS159PM1`	`61865`	40	from supplier
PhytoComm	Fo Shou	`G307HS159PM1`	`61866`	40	from supplier

Validation samples

A total of 23 740 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 *Fo Shou*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Fo Shou*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fo Shou	G307HS159PM1	61865†	20
PhytoComm	Fo Shou	G307HS159PM1	61866†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Fo Shou*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phytocomm	Fo Shou	44503	1
Phytocomm	Fo Shou	G307H0888321	1
phytocomm	Fo Shou	H0888021	1
PhytoComm	Fo Shou	H0888021	1

- 2047 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fo Shou* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fo Shou* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	4	2047

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4538 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61865	61865	0.00	9.61
61866	61866	0.00	9.64

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Fu Ling**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	50260-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fu Ling; Poriae cocos sclerotium

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Fu Ling	G200H1019623	62239	40	from supplier
PhytoComm	Fu Ling	G200H1019623	62240	40	from supplier

Validation samples

A total of 23 740 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 *Fu Ling*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Fu Ling*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fu Ling	G200H1019623	62239†	20
PhytoComm	Fu Ling	G200H1019623	62240†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 11 *Apo-Ident* customers from 5 batches from the substance/substance group *Fu Ling*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Fu Ling	421001902	1
Phyto Comm	Fu Ling	G200H1019522	1
Phytocomm	Fu Ling	G200H1019522	2
PhytoComm	Fu Ling	G200H1019221	3
PhytoComm	Fu Ling	G200H1019522	1
Phytocomm	Fu Ling	G200H1019221	4
PhytoComm	Fu Ling	G200H1019321	2
Phytocomm	Fu Ling	G200H1019321	1
Phytocomm	Fu Ling	g200h1019321	3

- 2033 spectra from 16 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fu Ling* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fu Ling* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	0	18	2032

The substance/substance group *Fu Ling* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9627 % (> 99.6888 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62239	62239	0.00	17.35
62240	62240	0.00	18.19

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Fu Pen Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60044-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fu Pen Zi; Rubi chingii fructus

Special notes

When selecting the *Fu Pen Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Fu Pen Zi	G213H1813621	61780	40	from supplier
PhytoComm	Fu Pen Zi	G213H1813621	61803	40	from supplier

Validation samples

A total of 23 740 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 *Fu Pen Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Fu Pen Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fu Pen Zi	G213H1813621	61780†	20
PhytoComm	Fu Pen Zi	G213H1813621	61803†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Fu Pen Zi*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Fu Pen Zi	g213h1813122	1
Phytocomm	Fu Pen Zi	G213H1813122	1
PhytoComm	Fu Pen Zi	H1813021	1

- 2048 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fu Pen Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fu Pen Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	3	1	2	2045

The substance/substance group *Fu Pen Zi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.8756 % (> 99.6029 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61780	61780	0.00	14.74
61803	61803	0.00	14.92

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Fu Xiao Mai**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60081-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fu Xiao Mai; Tritici aestivi semen levis

Special notes

When selecting the *Fu Xiao Mai* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Fu Xiao Mai	`G244HS021QM1`	`62183`	40	from supplier
PhytoComm	Fu Xiao Mai	`G244HS021QM1`	`62184`	40	from supplier

Validation samples

A total of 23 740 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 *Fu Xiao Mai*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Fu Xiao Mai*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fu Xiao Mai	G244HS021QM1	62183†	20
PhytoComm	Fu Xiao Mai	G244HS021QM1	62184†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Fu Xiao Mai*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phytocomm	Fu Xiao Mai	H1078021	1
Phytocomm	Fu Xiao Mai	G244H1078121	1
Phytocomm	Fu Xiao Mai	H1078021	1

- 2048 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fu Xiao Mai* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fu Xiao Mai* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	37	3	7409
Type C	0	0	3	2048

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	92.5000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4545 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62183	62183	0.00	4.37
62184	62184	0.00	4.40

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Fu Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	50884-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fu Zi; Aconiti lateralis radix praeparata; Aconiti radix lateralis praep.

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Fu Zi	G005H0801524	61728	40	from supplier
PhytoComm	Fu Zi	G005H0801524	62071	40	from supplier
PhytoComm	Fu Zi	G005H0801524	62072	40	from supplier
PhytoComm	Fu Zi	G005H0801624	62081	40	from supplier
PhytoComm	Fu Zi	G005H0801624	62082	40	from supplier
PhytoComm	Fu Zi	G005H0801723	62225	40	from supplier
PhytoComm	Fu Zi	G005H0801723	62226	40	from supplier

Validation samples

A total of 23 740 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 *Fu Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 3 different batches.

- 13 960 spectra from a total of 175 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 140 spectra from 7 reference samples of the substance/substance group *Fu Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fu Zi	G005H0801524	61728†	20
PhytoComm	Fu Zi	G005H0801524	62071†	20
PhytoComm	Fu Zi	G005H0801524	62072†	20
PhytoComm	Fu Zi	G005H0801624	62081†	20
PhytoComm	Fu Zi	G005H0801624	62082†	20
PhytoComm	Fu Zi	G005H0801723	62225†	20
PhytoComm	Fu Zi	G005H0801723	62226†	20

- 7309 spectra from a total of 178 batches from further 143 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 13 spectra from 7 *Apo-Ident* customers from 7 batches from the substance/substance group *Fu Zi*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phythocom	Fu Zi	goo5h0801122	1
Phytocomm	Fu Zi	161213fz	1
Phytocomm	Fu Zi	G005H0801524	1
Phytocomm	Fu Zi	G005H0801122	6
PhytoComm	Fu Zi	G005H0801122	1
Phytocomm	Fu Zi	g005h0801122	1
Phytocomm	Fu Zi	G005H0801322	1
phytocomm	Fu Zi	g005h0801322	1

- 2038 spectra from 17 *Apo-Ident* customers from a total of 967 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fu Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fu Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	13 960
Type B	0	140	0	7309
Type C	12	1	12	2026

The substance/substance group *Fu Zi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9477 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.8989 %)	100.0000 % (> 95.7143 %)
Type C	99.4603 % (> 99.1865 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61728	61728	0.00	9.83
62071	62071	0.00	13.29
62072	62072	0.00	13.36
62081	62081	0.00	11.20
62082	62082	0.00	11.44
62225	62225	0.00	13.55
62226	62226	0.00	12.83

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Gan Cao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60011-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gan Cao; Glycyrrhizae radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gan Cao	`G119H0521622`	`62145`	40	from supplier
PhytoComm	Gan Cao	`G119H0521622`	`62146`	40	from supplier

Validation samples

A total of 23 740 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 *Gan Cao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Gan Cao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gan Cao	G119H0521622	62145†	20
PhytoComm	Gan Cao	G119H0521622	62146†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 17 spectra from 9 *Apo-Ident* customers from 4 batches from the substance/substance group *Gan Cao*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Gan Cao	G119H0521522	7
Phytocomm	Gan Cao	G119H0521121	3
PhytoComm	Gan Cao	G119H0521121	5
Phytocomm	Gan Cao	g119h0521121	1
PhytoComm	Gan Cao	H0521923	1

- 2034 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gan Cao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gan Cao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	2	15	2034

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4522 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62145	62145	0.00	13.49
62146	62146	0.00	13.50

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Gan Jiang**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60077-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gan Jiang; Zingiberis rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gan Jiang	G252H1145622	62111	39	from supplier
PhytoComm	Gan Jiang	G252H1145622	62112	40	from supplier

Validation samples

A total of 23 740 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 *Gan Jiang*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 161 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Gan Jiang*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gan Jiang	G252H1145622	62111†	20
PhytoComm	Gan Jiang	G252H1145622	62112†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 8 *Apo-Ident* customers from 7 batches from the substance/substance group *Gan Jiang*.

- These include spectra of independent samples from 7 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Gan Jiang	G252H1145521	1
Phytocomm	Gan Jiang	g252h01145221	1
PhytoComm	Gan Jiang	G252H1145221	1
Caelo	Gan Jiang	G252H1145221	1
Phytocomm	Gan Jiang	G252H1145221	2
Phytocomm	Gan Jiang	H1145021	1
PhytoComm	Gan Jiang	H1145021	1
phythocom	Gan Jiang	G252H1145221	1
phythocom	Gan Jiang	252h1145021	1
phythocom	Gan Jiang	g252h1145221	1
phythocom	Gan Jiang	G25H1145221	1

- 2039 spectra from 17 *Apo-Ident* customers from a total of 967 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gan Jiang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gan Jiang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 161
Type B	0	40	0	7409
Type C	5	1	11	2034

The substance/substance group *Gan Jiang* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.4051 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.7766 % (> 99.5028 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62111	62111	0.00	8.46
62112	62112	0.00	8.56

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ge Gen**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60050-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ge Gen; Puerariae radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ge Gen	G206H1301621	61949	40	from supplier
PhytoComm	Ge Gen	G206H1301621	61950	40	from supplier

Validation samples

A total of 23 740 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 *Ge Gen*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Ge Gen*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ge Gen	G206H1301621	61949†	20
PhytoComm	Ge Gen	G206H1301621	61950†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 8 *Apo-Ident* customers from 5 batches from the substance/substance group *Ge Gen*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Ge Gen	161213gg	1
Phytocomm	Ge Gen	G206H1301422	2
phytocomm	Ge Gen	FA1301902	1
Phytocomm	Ge Gen	FA1301902	2
Phytocomm	Ge Gen	G206H1301221	2
PhytoComm	Ge Gen	FA1301902	1
PhytoComm	Ge Gen	G206H1301323	1

- 2041 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ge Gen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ge Gen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	10	2041

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61949	61949	0.00	23.22
61950	61950	0.00	23.78

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Gou Qi Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60094-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gou Qi Zi; Lycii chinensis fructus

Special notes

When selecting the *Gou Qi Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gou Qi Zi	G150H0913622	62243	40	from supplier
PhytoComm	Gou Qi Zi	G150H0913622	62244	40	from supplier

Validation samples

A total of 23 740 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 *Gou Qi Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Gou Qi Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gou Qi Zi	G150H0913622	62243†	20
PhytoComm	Gou Qi Zi	G150H0913622	62244†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Gou Qi Zi*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Gou Qi Zi	G150H0913422	3
phytocomm	Gou Qi Zi	G150H0913023	1
PhytoComm	Gou Qi Zi	G150H0913023	2
Phytocomm	Gou Qi Zi	G150H0913121	1
PhytoComm	Gou Qi Zi	G150H0913121	1
PhytoComm	Gou Qi Zi	G150H0913123	1
Phytocomm	Gou Qi Zi	g150h0913221	1
PhytoComm	Gou Qi Zi	G150H0913221	2

- 2039 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gou Qi Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gou Qi Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	4	1	11	2035

The substance/substance group *Gou Qi Zi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.8684 % (> 99.5946 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62243	62243	0.00	13.94
62244	62244	0.00	13.38

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Gu Sui Bu**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60225-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gu Sui Bu; Drynariae rhizoma

Special notes

When selecting the *Gu Sui Bu* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gu Sui Bu	G094H1011522	61714	40	from supplier

Validation samples

A total of 23 740 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 *Gu Sui Bu*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Gu Sui Bu*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gu Sui Bu	G094H1011522	61714†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Gu Sui Bu*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Gu Sui Bu	(G094)H1011221	1
PhytoComm	Gu Sui Bu	G094H1011023	2
Phytocomm	Gu Sui Bu	G094H1011023	1
Phytocomm	Gu Sui Bu	g094h1011023	1
Phytocomm	Gu Sui Bu	G094H1011221	2
PhytoComm	Gu Sui Bu	G094H1011221	1
Phytocomm	Gu Sui Bu	g094h1011221	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gu Sui Bu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gu Sui Bu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	0	0	9	2042

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.4526 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61714	61714	0.00	19.02

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Gua Lou**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60128-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gua Lou; Trichosanthis fructus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gua Lou	G241H1096521	61379	40	from supplier
PhytoComm	Gua Lou	G241H1096523	61787	40	from supplier
PhytoComm	Gua Lou	G241H1096523	61801	40	from supplier
PhytoComm	Gua Lou	G241H1096523	61877	40	from supplier
PhytoComm	Gua Lou	G241H1096621	61913	40	from supplier
PhytoComm	Gua Lou	G241H1096621	61914	40	from supplier

Validation samples

A total of 23 740 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 *Gua Lou*. These samples are listed above in the section *calibration samples*. The reference samples originate from 3 different batches.

- 14 000 spectra from a total of 175 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 168 spectra from 7 reference samples of the substance/substance group *Gua Lou*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gua Lou	G241H1096521	61379†	20
PhytoComm	Gua Lou	G241H1096523	61787†	20
PhytoComm	Gua Lou	G241H1096523	61801†	20
PhytoComm	Gua Lou	G241H1096523	61877†	19
PhytoComm	Gua Lou	G241H1096523	61878	49
PhytoComm	Gua Lou	G241H1096621	61913†	20
PhytoComm	Gua Lou	G241H1096621	61914†	20

- 7281 spectra from a total of 178 batches from further 143 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 11 spectra from 6 *Apo-Ident* customers from 6 batches from the substance/substance group *Gua Lou*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Gua Lou	G241H1096521	1
phytocomm	Gua Lou	G241H1096121	1
Phytocomm	Gua Lou	G241H1096121	1
PhytoComm	Gua Lou	G241H1096121	2
Phytocomm	Gua Lou	G241H1096321	1
PhytoComm	Gua Lou	G241H1096321	1
Phytocomm	Gua Lou	g241h1096321	1
PhytoComm	Gua Lou	G241H1096322	2
Phytocomm	Gua Lou	H1096922	1

- 2040 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gua Lou* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gua Lou* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 000
Type B	0	168	0	7281
Type C	3	4	7	2037

The substance/substance group *Gua Lou* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9477 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.8989 %)	100.0000 % (> 96.4286 %)
Type C	99.8752 % (> 99.6014 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61379	61379	0.00	16.33
61787	61787	0.00	16.40
61801	61801	0.00	16.51
61877	61877	0.00	12.31
61913	61913	0.00	9.19
61914	61914	0.00	8.74

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Gua Lou Ren**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60052-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gua Lou Ren; Trichosanthis semen

Special notes

When selecting the *Gua Lou Ren* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gua Lou Ren	G243H1095621	61775	40	from supplier
PhytoComm	Gua Lou Ren	G243H1095621	61809	40	from supplier

Validation samples

A total of 23 740 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 *Gua Lou Ren*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Gua Lou Ren*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gua Lou Ren	G243H1095621	61775†	20
PhytoComm	Gua Lou Ren	G243H1095621	61809†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Gua Lou Ren*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Gua Lou Ren	G243H1095421	1
Phytocomm	Gua Lou Ren	G243H1095123	1
Phytocomm	Gua Lou Ren	g243h1095123	1

- 2048 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gua Lou Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gua Lou Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	3	2048

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4545 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61775	61775	0.00	15.57
61809	61809	0.00	14.89

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Guang Huo Xiang**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	61079-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Guang Huo Xiang; Pogostemonis herba

Special notes

When selecting the *Guang Huo Xiang* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Guang Huo Xiang	G007H2005621	62037	40	from supplier
PhytoComm	Guang Huo Xiang	G007H2005621	62038	40	from supplier

Validation samples

A total of 23 740 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 *Guang Huo Xiang*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Guang Huo Xiang*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Guang Huo Xiang	G007H2005621	62037†	20
PhytoComm	Guang Huo Xiang	G007H2005621	62038†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 1 batches from the substance/substance group *Guang Huo Xiang*.

- These include spectra of independent samples from 1 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Guang Huo Xiang	G007H2005521	2

- 2049 spectra from 17 *Apo-Ident* customers from a total of 973 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Guang Huo Xiang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Guang Huo Xiang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	2	2049

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4559 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62037	62037	0.00	24.18
62038	62038	0.00	24.50

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Gui Ban Jiao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60126-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gui Ban Jiao; Colla carapax et plastrum chrysemys

Special notes

When selecting the *Gui Ban Jiao* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gui Ban Jiao	G326HS330OV1	61725	40	from supplier

Validation samples

A total of 23 740 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 *Gui Ban Jiao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Gui Ban Jiao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gui Ban Jiao	G326HS330OV1	61725†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 *Gui Ban Jiao*.

- These include spectra of independent samples from 1 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Gui Ban Jiao	G326H2205221	1

- 2050 spectra from 17 *Apo-Ident* customers from a total of 973 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gui Ban Jiao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gui Ban Jiao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	0	0	1	2050

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.4601 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61725	61725	0.00	23.24

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Gui Zhi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60189-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gui Zhi; Cinnamomi cassiae ramulus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gui Zhi	G070H1001523	61698	40	from supplier
PhytoComm	Gui Zhi	G070H1001621	61777	40	from supplier
PhytoComm	Gui Zhi	G070H1001621	61815	40	from supplier
PhytoComm	Gui Zhi	G070H1001621	61873	40	from supplier
PhytoComm	Gui Zhi	G070H1001621	61874	40	from supplier
PhytoComm	Gui Zhi	G070H1001621	62065	40	from supplier
PhytoComm	Gui Zhi	G070H1001621	62066	40	from supplier
PhytoComm	Gui Zhi	G070H1001624	62103	40	from supplier
PhytoComm	Gui Zhi	G070H1001624	62104	40	from supplier

Validation samples

A total of 23 740 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 *Gui Zhi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 3 different batches.

- 13 880 spectra from a total of 175 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 180 spectra from 9 reference samples of the substance/substance group *Gui Zhi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gui Zhi	G070H1001523	61698†	20
PhytoComm	Gui Zhi	G070H1001621	61777†	20
PhytoComm	Gui Zhi	G070H1001621	61815†	20
PhytoComm	Gui Zhi	G070H1001621	61873†	20
PhytoComm	Gui Zhi	G070H1001621	61874†	20
PhytoComm	Gui Zhi	G070H1001621	62065†	20
PhytoComm	Gui Zhi	G070H1001621	62066†	20
PhytoComm	Gui Zhi	G070H1001624	62103†	20
PhytoComm	Gui Zhi	G070H1001624	62104†	20

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

- 7269 spectra from a total of 178 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 15 spectra from 8 *Apo-Ident* customers from 5 batches from the substance/substance group *Gui Zhi*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Gui Zhi	G070H1001523	2
Phytocomm	Gui Zhi	G070H1001221	2
PhytoComm	Gui Zhi	G070H1001221	1
Phytocomm	Gui Zhi	g070h1001422	1
Phytocomm	Gui Zhi	G070H100422	1
Phytocomm	Gui Zhi	H1001022	5
PhytoComm	Gui Zhi	H1001022	3

- 2036 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gui Zhi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gui Zhi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	13 880
Type B	0	180	0	7269
Type C	6	3	12	2030

The substance/substance group *Gui Zhi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9476 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.8988 %)	100.0000 % (> 96.6667 %)
Type C	99.6422 % (> 99.3684 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61698	61698	0.00	10.72
61777	61777	0.00	8.67
61815	61815	0.00	9.14
61873	61873	0.00	12.38
61874	61874	0.00	12.21
62065	62065	0.00	14.59
62066	62066	0.00	13.91
62103	62103	0.00	15.16
62104	62104	0.00	14.80

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**He Huan Pi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60175-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

He Huan Pi; Albiziae cortex; Albiziae julibrissini cortex

Special notes

When selecting the *He Huan Pi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	He Huan Pi	G010H0635622	62101	40	from supplier
PhytoComm	He Huan Pi	G010H0635622	62102	40	from supplier

Validation samples

A total of 23 740 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 *He Huan Pi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *He Huan Pi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	He Huan Pi	G010H0635622	62101†	20
PhytoComm	He Huan Pi	G010H0635622	62102†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 8 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *He Huan Pi*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	He Huan Pi	G010H0635221	1
PhytoComm	He Huan Pi	G010H0635221	2
Phytocomm	He Huan Pi	g010h0635221	1
PhytoComm	He Huan Pi	G010H0635321	1
Phytocomm	He Huan Pi	G010H0635423	1
PhytoComm	He Huan Pi	H0635021	2

- 2043 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *He Huan Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *He Huan Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	8	2043

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4528 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62101	62101	0.00	10.44
62102	62102	0.00	10.14

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Hong Jing Tian**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60031-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hong Jing Tian; Rhodiolae crenulatae radix

Special notes

When selecting the *Hong Jing Tian* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Hong Jing Tian	`G237H0906621`	`61911`	40	from supplier
PhytoComm	Hong Jing Tian	`G237H0906621`	`61912`	40	from supplier

Validation samples

A total of 23 740 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 *Hong Jing Tian*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Hong Jing Tian*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Hong Jing Tian	G237H0906621	61911†	20
PhytoComm	Hong Jing Tian	G237H0906621	61912†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 3 batches from the substance/substance group *Hong Jing Tian*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Hong Jing Tian	G237H0906221	2
Phytocomm	Hong Jing Tian	G237H0906221	2
Phytocomm	Hong Jing Tian	G237H0906321	1
Herbasinica	Hong Jing Tian	H0906021	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hong Jing Tian* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hong Jing Tian* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14160
Type B	0	40	0	7409
Type C	0	0	6	2045

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4531 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61911	61911	0.00	15.80
61912	61912	0.00	15.90

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Hou Po**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	50289-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hou Po; Magnoliae officinalis cortex

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Hou Po	G154H0917423	61387	40	from supplier
PhytoComm	Hou Po	G154H0917521	61782	40	from supplier
PhytoComm	Hou Po	G154H0917521	61826	40	from supplier

Validation samples

A total of 23 740 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 *Hou Po*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 120 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 60 spectra from 3 reference samples of the substance/substance group *Hou Po*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Hou Po	G154H0917423	61387†	20
PhytoComm	Hou Po	G154H0917521	61782†	20
PhytoComm	Hou Po	G154H0917521	61826†	20

- 7389 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 6 spectra from 5 *Apo-Ident* customers from 2 batches from the substance/substance group *Hou Po*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Hou Po	G154H0917222	1
Phytocomm	Hou Po	G154H0917222	1
phytocomm	Hou Po	H0917022	1
PhytoComm	Hou Po	H0917022	1
Phytocomm	Hou Po	H0917022	2

- 2045 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hou Po* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hou Po* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 120
Type B	0	60	0	7389
Type C	7	0	6	2038

The substance/substance group *Hou Po* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.8992 %)	100.0000 % (> 90.0000 %)
Type C	99.7281 % (> 99.4547 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61387	61387	0.00	14.80
61782	61782	0.00	12.16
61826	61826	0.00	12.15

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Huai Hua**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60120-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Huai Hua; Sophorae japonicae flos

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Huai Hua	G263H1423521	61891	40	from supplier
PhytoComm	Huai Hua	G263H1423521	61892	40	from supplier
PhytoComm	Huai Hua	G263H1423521	62153	40	from supplier
PhytoComm	Huai Hua	G263H1423521	62154	40	from supplier

Validation samples

A total of 23 740 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 *Huai Hua*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Huai Hua*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huai Hua	G263H1423521	61891†	20
PhytoComm	Huai Hua	G263H1423521	61892†	20
PhytoComm	Huai Hua	G263H1423521	62153†	20
PhytoComm	Huai Hua	G263H1423521	62154†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 6 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Huai Hua*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Huai Hua	G263H1423121	1
Phytocomm	Huai Hua	G263H1423421	1
PhytoComm	Huai Hua	G263H1423121	2
PhytoComm	Huai Hua	G263H143121	1
phythocom	Huai Hua	g263h1423121	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Huai Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huai Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 080
Type B	0	80	0	7369
Type C	1	3	3	2044

The substance/substance group *Huai Hua* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	99.9534 % (> 99.6799 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61891	61891	0.00	16.67
61892	61892	0.00	17.16
62153	62153	0.00	22.80
62154	62154	0.00	22.03

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Huang Bo**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60057-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Huang Bo; Phellodendri cortex chinensis

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Huang Bo	G188H1203622	61953	40	from supplier
PhytoComm	Huang Bo	G188H1203622	61954	40	from supplier

Validation samples

A total of 23 740 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 *Huang Bo*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Huang Bo*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huang Bo	G188H1203622	61953†	20
PhytoComm	Huang Bo	G188H1203622	61954†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 15 spectra from 9 *Apo-Ident* customers from 5 batches from the substance/substance group *Huang Bo*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Huang Bo	G188H1203123	2
Phytocomm	Huang Bo	G188H1203321	4
Phytocomm	Huang Bo	161213hb	1
Phytocomm	Huang Bo	G188H1203123	4
Phytocomm	Huang Bo	g188h1203123	1
PhytoComm	Huang Bo	G188H1203321	2
Phytocomm	Huang Bo	h1203022	1

- 2036 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Huang Bo* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huang Bo* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	15	2036

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4523 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61953	61953	0.00	11.29
61954	61954	0.00	10.97

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Huang Jing**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60108-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Huang Jing; Polygonati rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Huang Jing	`G196H1206522`	`61951`	40	from supplier
PhytoComm	Huang Jing	`G196H1206522`	`61952`	40	from supplier

Validation samples

A total of 23 740 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 *Huang Jing*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Huang Jing*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huang Jing	G196H1206522	61951†	20
PhytoComm	Huang Jing	G196H1206522	61952†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Huang Jing*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phytocomm	Huang Jing	FA1206822	1
ChinaMedica	Huang Jing	G196H1206121	1
Phytocomm	Huang Jing	G196H1206121	2
PhytoComm	Huang Jing	G196H1206121	1
Phytocomm	Huang Jing	g196h1206121	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Huang Jing* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huang Jing* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	8	0	6	2037

The substance/substance group *Huang Jing* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.3870 % (> 99.1135 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61951	61951	0.00	13.18
61952	61952	0.00	12.92

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Huang Lian**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60219-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Huang Lian; Coptidis rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Huang Lian	G079H1205521	61729	40	from supplier
PhytoComm	Huang Lian	G079H1205621	61776	40	from supplier
PhytoComm	Huang Lian	G079H1205621	61819	40	from supplier
PhytoComm	Huang Lian	G079H1205622	62091	40	from supplier
PhytoComm	Huang Lian	G079H1205622	62092	40	from supplier

Validation samples

A total of 23 740 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 *Huang Lian*. These samples are listed above in the section *calibration samples*. The reference samples originate from 3 different batches.

- 14 040 spectra from a total of 175 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 100 spectra from 5 reference samples of the substance/substance group *Huang Lian*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huang Lian	G079H1205521	61729†	20
PhytoComm	Huang Lian	G079H1205621	61776†	20
PhytoComm	Huang Lian	G079H1205621	61819†	20
PhytoComm	Huang Lian	G079H1205622	62091†	20
PhytoComm	Huang Lian	G079H1205622	62092†	20

- 7349 spectra from a total of 178 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 17 spectra from 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Huang Lian*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Huang Lian	FA1205702	1
Phytocomm	Huang Lian	G079H1205021	1
Phytocomm	Huang Lian	G079H1205321	2
PhytoComm	Huang Lian	G079H1205321	5
Phytocomm	Huang Lian	g079h1205321	1
Phytocomm	Huang Lian	G079H1205521	2
PhytoComm	Huang Lian	G079H1205521	2
PhytoComm	Huang Lian	H1205021	2
Phytocomm	Huang Lian	H1205021	1

- 2034 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Huang Lian* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huang Lian* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 040
Type B	0	100	0	7349
Type C	0	5	12	2034

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9477 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.4522 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61729	61729	0.00	45.13
61776	61776	0.00	47.00
61819	61819	0.00	48.43
62091	62091	0.00	44.78
62092	62092	0.00	44.92

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Huang Qi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60154-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Huang Qi; Astragali membranacei radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Huang Qi	G040H1202721	62227	40	from supplier
PhytoComm	Huang Qi	G040H1202721	62228	40	from supplier

Validation samples

A total of 23 740 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 *Huang Qi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Huang Qi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huang Qi	G040H1202721	62227†	20
PhytoComm	Huang Qi	G040H1202721	62228†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 24 spectra from 8 *Apo-Ident* customers from 8 batches from the substance/substance group *Huang Qi*.

- These include spectra of independent samples from 8 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Huang Qi	G040H1202423	1
Phytocomm	Huang Qi	G040H1202521	2
PhytoComm	Huang Qi	G040H1202621	1
PhytoComm	Huang Qi	G040H1202222	3
Phytocomm	Huang Qi	G040H1202222	5
Caelo	Huang Qi	g040h1202222	1
PhytoComm	Huang Qi	G040H1202321	2
Phytocomm	Huang Qi	G040H1202321	2
Phytocomm	Huang Qi	g040h1202321	2
PhytoComm	Huang Qi	H1202021	1
Phytocomm	Huang Qi	H1202021	4

- 2027 spectra from 17 *Apo-Ident* customers from a total of 966 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Huang Qi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Huang Qi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	3	14	10	2024

The substance/substance group *Huang Qi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.8031 % (> 99.5291 %)	58.3333 % (> 45.8333 %)

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
62227	62227	0.00	11.51
62228	62228	0.00	11.03

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Jiang Huang**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60181-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Jiang Huang; Curcumae longae rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Jiang Huang	`G085H1716422`	`61683`	40	from supplier

Validation samples

A total of 23 740 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 *Jiang Huang*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Jiang Huang*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jiang Huang	G085H1716422	61683†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 8 *Apo-Ident* customers from 4 batches from the substance/substance group *Jiang Huang*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Jiang Huang	G085H1716321	2
Phytocomm	Jiang Huang	G085H1716422	3
PhytoComm	Jiang Huang	G085H1716422	1
phytocomm	Jiang Huang	G085H1716022	1
Phytocomm	Jiang Huang	G085H1716022	1
PhytoComm	Jiang Huang	G085H1716022	1
PhytoComm	Jiang Huang	G085H1716122	2
Phytocomm	Jiang Huang	G085H1716122	1

- 2039 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Jiang Huang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jiang Huang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	1	7	5	2038

The substance/substance group *Jiang Huang* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	99.9067 % (> 99.6329 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61683	61683	0.00	20.34

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Jiao Gu Lan**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60332-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Jiao Gu Lan; Gynostemma herba

Special notes

When selecting the *Jiao Gu Lan* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Jiao Gu Lan	G065FB1276621	62013	40	from supplier
PhytoComm	Jiao Gu Lan	G065FB1276621	62014	40	from supplier

Validation samples

A total of 23 740 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 *Jiao Gu Lan*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Jiao Gu Lan*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jiao Gu Lan	G065FB1276621	62013†	20
PhytoComm	Jiao Gu Lan	G065FB1276621	62014†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 7 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Jiao Gu Lan*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Jiao Gu Lan	G065FB1276421	3
Phytocomm	Jiao Gu Lan	G065F-B1276121	1
Herbasin	Jiao Gu Lan	G065FB1276121	1
Herbasinica	Jiao Gu Lan	G065F-B1276121	1
PhytoComm	Jiao Gu Lan	G065H1276922	1

- 2044 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Jiao Gu Lan* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jiao Gu Lan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	0	7	2043

The substance/substance group *Jiao Gu Lan* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9627 % (> 99.6891 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62013	62013	0.00	9.72
62014	62014	0.00	10.30

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Jie Geng**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60034-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Jie Geng; Platycodi grandiflori radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Jie Geng	G193H1015621	61931	40	from supplier
PhytoComm	Jie Geng	G193H1015621	61932	40	from supplier
PhytoComm	Jie Geng	G193H1015721	62247	40	from supplier
PhytoComm	Jie Geng	G193H1015721	62248	40	from supplier

Validation samples

A total of 23 740 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 *Jie Geng*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Jie Geng*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jie Geng	G193H1015621	61931†	20
PhytoComm	Jie Geng	G193H1015621	61932†	20
PhytoComm	Jie Geng	G193H1015721	62247†	20
PhytoComm	Jie Geng	G193H1015721	62248†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 15 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Jie Geng*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Jie Geng	G193H1015521	3
PhytoComm	Jie Geng	G193H1015024	2
Phytocomm	Jie Geng	G193H1015024	3
Phytocomm	Jie Geng	G193H1015025	2
phytocomm	Jie Geng	G193H1015025	1
Phytocomm	Jie Geng	G193H1015221	3
Phytocomm	Jie Geng	g193h1015221	1

- 2036 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Jie Geng* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jie Geng* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 080
Type B	0	79	1	7369
Type C	2	1	14	2034

The substance/substance group *Jie Geng* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	98.7500 % (> 95.0000 %)
Type C	99.8934 % (> 99.6195 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61931	61931	0.00	7.66
61932	61932	0.00	7.03
62247	62247	0.00	6.67
62248	62248	0.00	6.53

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Jin Yin Hua**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60350-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Jin Yin Hua; Lonicerae japonicae flos

Special notes

When selecting the *Jin Yin Hua* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Jin Yin Hua	G145HS311QG1	62189	40	from supplier
PhytoComm	Jin Yin Hua	G145HS311QG1	62190	40	from supplier

Validation samples

A total of 23 740 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 *Jin Yin Hua*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Jin Yin Hua*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jin Yin Hua	G145HS311QG1	62189†	20
PhytoComm	Jin Yin Hua	G145HS311QG1	62190†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Jin Yin Hua*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Jin Yin Hua	G145H0845021	1
Phytocomm	Jin Yin Hua	G145H0845022	4
Phytocomm	Jin Yin Hua	G145H0845321	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Jin Yin Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jin Yin Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	0	6	2044

The substance/substance group *Jin Yin Hua* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9254 % (> 99.6519 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62189	62189	0.00	15.89
62190	62190	0.00	15.41

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Jing Jie**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60088-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Jing Jie; Schizonepetae tenuifoliae herba

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Jing Jie	G221H1038621	61923	40	from supplier
PhytoComm	Jing Jie	G221H1038621	61924	40	from supplier
PhytoComm	Jing Jie	G221H1038621	62055	40	from supplier
PhytoComm	Jing Jie	G221H1038621	62056	40	from supplier

Validation samples

A total of 23 740 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 *Jing Jie*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Jing Jie*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jing Jie	G221H1038621	61923†	20
PhytoComm	Jing Jie	G221H1038621	61924†	20
PhytoComm	Jing Jie	G221H1038621	62055†	20
PhytoComm	Jing Jie	G221H1038621	62056†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 11 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Jing Jie*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phytocomm	Jing Jie	G221H1038121	2
Sino Phyto	Jing Jie	G221H1038121	1
PhytoComm	Jing Jie	G221H1038121	1
Phytocomm	Jing Jie	G221H1038221	4
PhytoComm	Jing Jie	G221H1038221	1
Phytocomm	Jing Jie	g221h1038221	1
PhytoComm	Jing Jie	H1038021	1

- 2040 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Jing Jie* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Jing Jie* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 080
Type B	0	80	0	7369
Type C	7	0	11	2033

The substance/substance group *Jing Jie* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	99.6383 % (> 99.3645 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61923	61923	0.00	6.95
61924	61924	0.00	7.58
62055	62055	0.00	7.13
62056	62056	0.00	7.05

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ju Hua**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60232-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ju Hua; Chrysanthemi flos

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ju Hua	G064H1231521	62023	40	from supplier
PhytoComm	Ju Hua	G064H1231521	62024	40	from supplier

Validation samples

A total of 23 740 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 *Ju Hua*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Ju Hua*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ju Hua	G064H1231521	62023†	20
PhytoComm	Ju Hua	G064H1231521	62024†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 2 batches from the substance/substance group *Ju Hua*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Ju Hua	G064H1231421	2
PhytoComm	Ju Hua	G064H1231421	1
PhytoComm	Ju Hua	G064H1231021	2

- 2046 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ju Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ju Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	4	1	2046

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4534 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62023	62023	0.00	19.49
62024	62024	0.00	19.41

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ku Shen**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60112-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ku Shen; Sophorae flavescentis radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ku Shen	`G233H0908521`	`61927`	40	from supplier
PhytoComm	Ku Shen	`G233H0908521`	`61928`	40	from supplier

Validation samples

A total of 23 740 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 *Ku Shen*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Ku Shen*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ku Shen	G233H0908521	61927†	20
PhytoComm	Ku Shen	G233H0908521	61928†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 8 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Ku Shen*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
china medica 14.06.2013	Ku Shen	210013	1
Phytocomm	Ku Shen	FA0908901	1
Phytocomm	Ku Shen	G233H0908121	4
PhytoComm	Ku Shen	G233H0908121	1
Phytocomm	Ku Shen	h0908121	1

- 2043 spectra from 16 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ku Shen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ku Shen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	8	2043

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4528 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61927	61927	0.00	23.23
61928	61928	0.00	22.91

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Kuan Dong Hua**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60035-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Kuan Dong Hua; Farfarae flos; Tussilaginis farfarae flos

Special notes

When selecting the *Kuan Dong Hua* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Kuan Dong Hua	G276H1219521	61660	40	from supplier

Validation samples

A total of 23 740 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 *Kuan Dong Hua*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Kuan Dong Hua*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Kuan Dong Hua	G276H1219521	61660†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Kuan Dong Hua*.

- These include spectra of independent samples from 1 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Kuan Dong Hua	H1219921	2

- 2049 spectra from 17 *Apo-Ident* customers from a total of 973 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Kuan Dong Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Kuan Dong Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	10	0	2	2039

The substance/substance group *Kuan Dong Hua* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	99.5080 % (> 99.2360 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61660	61660	0.00	15.54

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Lai Fu Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60067-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lai Fu Zi; Raphani sativi semen

Special notes

When selecting the *Lai Fu Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Lai Fu Zi	G209H1220621	61959	40	from supplier
PhytoComm	Lai Fu Zi	G209H1220621	61960	40	from supplier

Validation samples

A total of 23 740 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 *Lai Fu Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Lai Fu Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Lai Fu Zi	G209H1220621	61959†	20
PhytoComm	Lai Fu Zi	G209H1220621	61960†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Lai Fu Zi*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Lai Fu Zi	G209H1220022	2
PhytoComm	Lai Fu Zi	G209H1220022	1
Phytocomm	Lai Fu Zi	G209H1220221	1
PhytoComm	Lai Fu Zi	G209H1220321	1
Phytocomm	Lai Fu Zi	G209H1220321	1
Herbasin	Lai Fu Zi	g209h1220321	1
PhytoComm	Lai Fu Zi	H1220922	2

- 2042 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lai Fu Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lai Fu Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	9	2042

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4526 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61959	61959	0.00	33.79
61960	61960	0.00	33.95

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Lian Qiao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60146-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lian Qiao; Forsythiae fructus; Forsythiae suspensae fructus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Lian Qiao	`G105H1132721`	`62231`	40	from supplier
PhytoComm	Lian Qiao	`G105H1132721`	`62232`	40	from supplier

Validation samples

A total of 23 740 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 *Lian Qiao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Lian Qiao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Lian Qiao	G105H1132721	62231†	20
PhytoComm	Lian Qiao	G105H1132721	62232†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 7 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Lian Qiao*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Lian Qiao	G105H1132221	2
PhytoComm	Lian Qiao	G105H1132221	1
Phytocomm	Lian Qiao	G105H1132521	1
PhytoComm	Lian Qiao	H1132022	1
Phytocomm	Lian Qiao	H1132022	1
PhytoComm	Lian Qiao	G105H1132321	1

- 2044 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lian Qiao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lian Qiao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	7	2044

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4529 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62231	62231	0.00	27.02
62232	62232	0.00	26.89

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Lian Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60248-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lian Zi; Nelumbinis semen

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Lian Zi	`G171HS312QM1`	`62197`	40	from supplier
PhytoComm	Lian Zi	`G171HS312QM1`	`62198`	39	from supplier

Validation samples

A total of 23 740 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 *Lian Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 161 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Lian Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Lian Zi	G171HS312QM1	62197†	20
PhytoComm	Lian Zi	G171HS312QM1	62198†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 *Lian Zi*.

- These include spectra of independent samples from 1 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Lian Zi	411502701	1

- 2050 spectra from 17 *Apo-Ident* customers from a total of 973 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	1	77	2	14 160
Type B	13	27	13	7396
Type C	2	0	1	2048

The substance/substance group *Lian Zi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	99.9941 % (> 99.9681 %)	97.4684 % (> 93.6709 %)
Type B	99.8495 % (> 99.7992 %)	67.5000 % (> 60.0000 %)
Type C	99.5025 % (> 99.2325 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62197	62197	0.00	3.68
62198	62198	0.00	4.23

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Long Dan (Cao)**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60227-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Long Dan (Cao); Gentianae longdancao radix; Gentianae scabrae radix

Special notes

When selecting the *Long Dan (Cao)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Long Dan (Cao)	G112H1705621	62123	40	from supplier
PhytoComm	Long Dan (Cao)	G112H1705621	62124	41	from supplier

Validation samples

A total of 23 740 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 81 spectra of 2 reference samples from the substance/substance group *Long Dan (Cao)*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 159 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Long Dan (Cao)*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Long Dan (Cao)	G112H1705621	62123†	20
PhytoComm	Long Dan (Cao)	G112H1705621	62124†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 8 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Long Dan (Cao)*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Long Dan (Cao)	G112H1705321	3
Phytocomm	Long Dan (Cao)	g112h1705022	1
PhytoComm	Long Dan (Cao)	G112H1705022	3
Phytocomm	Long Dan (Cao)	G112H1705022	1

- 2043 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	81	0	14 159
Type B	0	40	0	7409
Type C	5	0	8	2038

The substance/substance group *Long Dan (Cao)* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5926 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.7564 % (> 99.4828 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62123	62123	0.00	9.84
62124	62124	0.00	9.31

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Long Yan Rou**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60463-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Long Yan Rou; Euphoriae longanae arillus; Longan Arillus

Special notes

When selecting the *Long Yan Rou* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Long Yan Rou	G144HS324PW1	62203	40	from supplier
PhytoComm	Long Yan Rou	G144HS324PW1	62204	40	from supplier

Validation samples

A total of 23 740 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 *Long Yan Rou*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Long Yan Rou*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Long Yan Rou	G144HS324PW1	62203†	20
PhytoComm	Long Yan Rou	G144HS324PW1	62204†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 2 batches from the substance/substance group *Long Yan Rou*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Long Yan Rou	G144H1708221	1
PhytoComm	Long Yan Rou	G144H1708221	1
phytocomm	Long Yan Rou	H1708922	2
PhytoComm	Long Yan Rou	H1708922	2

- 2045 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Long Yan Rou* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Long Yan Rou* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	6	2045

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4531 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62203	62203	0.00	11.13
62204	62204	0.00	12.22

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Lu Lu Tong**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60240-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lu Lu Tong; Liquidambaris fructus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Lu Lu Tong	G142H1336622	62001	40	from supplier
PhytoComm	Lu Lu Tong	G142H1336622	62002	40	from supplier

Validation samples

A total of 23 740 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 *Lu Lu Tong*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Lu Lu Tong*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Lu Lu Tong	G142H1336622	62001†	20
PhytoComm	Lu Lu Tong	G142H1336622	62002†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Lu Lu Tong*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Lu Lu Tong	G142GH1336022	1
Phytocomm	Lu Lu Tong	G142H1336122	1
Herbasinica	Lu Lu Tong	G142H1336122	2
PhytoComm	Lu Lu Tong	g142h1336122	1
PhytoComm	Lu Lu Tong	G142H1336122	1
Phytocomm	Lu Lu Tong	G142H1336521	2
Phytocomm	Lu Lu Tong	G142H1336321	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lu Lu Tong* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lu Lu Tong* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	9	2042

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4526 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62001	62001	0.00	13.19
62002	62002	0.00	13.52

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ma Huang**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	50283-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ma Huang; Ephedrae herba

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ma Huang	G097H1101522	61684	40	from supplier
PhytoComm	Ma Huang	G097H1101623	62147	40	from supplier
PhytoComm	Ma Huang	G097H1101623	62148	40	from supplier

Validation samples

A total of 23 740 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 *Ma Huang*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 120 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 60 spectra from 3 reference samples of the substance/substance group *Ma Huang*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ma Huang	G097H1101522	61684†	20
PhytoComm	Ma Huang	G097H1101623	62147†	20
PhytoComm	Ma Huang	G097H1101623	62148†	20

- 7389 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 8 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Ma Huang*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Ma Huang	G097H1101522	2
Phytocomm	Ma Huang	G097H1101223	3
PhytoComm	Ma Huang	H1101023	2
Phytocomm	Ma Huang	H1101023	1

- 2043 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ma Huang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ma Huang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 120
Type B	0	60	0	7389
Type C	0	2	6	2043

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.8992 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.4528 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61684	61684	0.00	39.28
62147	62147	0.00	33.08
62148	62148	0.00	33.84

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ma Huang Gen**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60063-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ma Huang Gen; Ephedrae radix

Special notes

When selecting the *Ma Huang Gen* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ma Huang Gen	`G278HS393OV1`	`61727`	40	from supplier

Validation samples

A total of 23 740 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 *Ma Huang Gen*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Ma Huang Gen*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ma Huang Gen	G278HS393OV1	61727†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Ma Huang Gen*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phythocom	Ma Huang Gen	g278h1102121	1
phytocomm	Ma Huang Gen	h1102021	1
PhytoComm	Ma Huang Gen	G278H1102121	1
Herbasin	Ma Huang Gen	G278H1102121	2
Phytocomm	Ma Huang Gen	G278H1102121	2
Herbasin	Ma Huang Gen	H1102021	1
Phytocomm	Ma Huang Gen	H1102021	1
PhytoComm	Ma Huang Gen	H1102021	1

- 2041 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ma Huang Gen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ma Huang Gen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	5	20	0	7424
Type C	0	0	10	2041

The substance/substance group *Ma Huang Gen* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	99.9132 % (> 99.8633 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61727	61727	0.00	5.25

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Mai Men Dong**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60024-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mai Men Dong; Ophiopogonis radix

Special notes

When selecting the *Mai Men Dong* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Mai Men Dong	G176H1118621	61945	40	from supplier
PhytoComm	Mai Men Dong	G176H1118621	61946	40	from supplier
PhytoComm	Mai Men Dong	G176H1118622	62113	40	from supplier
PhytoComm	Mai Men Dong	G176H1118622	62114	40	from supplier

Validation samples

A total of 23 740 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 *Mai Men Dong*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Mai Men Dong*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mai Men Dong	G176H1118621	61945†	20
PhytoComm	Mai Men Dong	G176H1118621	61946†	20
PhytoComm	Mai Men Dong	G176H1118622	62113†	20
PhytoComm	Mai Men Dong	G176H1118622	62114†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 11 spectra from 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Mai Men Dong*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Mai Men Dong	G176H1118322	1
Phytocomm	Mai Men Dong	G176H1118521	3
Phytocomm	Mai Men Dong	1206mmd	1
Phytocomm	Mai Men Dong	G176H1118221	1
Phytocomm	Mai Men Dong	g176h1118221	1
Phytocomm	Mai Men Dong	H1118021	2
PhytoComm	Mai Men Dong	H1118021	2

- 2040 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mai Men Dong* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mai Men Dong* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 080
Type B	0	80	0	7369
Type C	0	3	8	2040

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61945	61945	0.00	15.86
61946	61946	0.00	15.67
62113	62113	0.00	12.35
62114	62114	0.00	11.37

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Mai Ya**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60210-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mai Ya; Hordei vulgaris fructus germinatus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Mai Ya	G123H1119521	61745	40	from supplier
PhytoComm	Mai Ya	G123H1119521	62069	40	from supplier

Validation samples

A total of 23 740 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 *Mai Ya*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 91 spectra from 3 reference samples of the substance/substance group *Mai Ya*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mai Ya	G123H1119521	61745†	20
PhytoComm	Mai Ya	G123H1119521	62069†	20
PhytoComm	Mai Ya	G123H1119521	62070	51

- 7358 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 8 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Mai Ya*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Mai Ya	G123H1119521	1
Phytocomm	Mai Ya	G123H1119022	1
Phytocomm	Mai Ya	g123h1119022	1
PhytoComm	Mai Ya	G123H1119022	1
PhytoComm	Mai Ya	G123H1119122	2
Phytocomm	Mai Ya	G123H1119122	1
PhytoComm	Mai Ya	H1119922	1

- 2043 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mai Ya* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mai Ya* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	87	4	7358
Type C	3	1	7	2040

The substance/substance group *Mai Ya* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8990 %)	95.6044 % (> 92.3077 %)
Type C	99.8220 % (> 99.5484 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61745	61745	0.00	14.37
62069	62069	0.00	9.77

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Man Jing Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60025-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Man Jing Zi; Viticis fructus

Special notes

When selecting the *Man Jing Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Man Jing Zi	G250H1505622	61899	40	from supplier
PhytoComm	Man Jing Zi	G250H1505622	61900	40	from supplier

Validation samples

A total of 23 740 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 *Man Jing Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Man Jing Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Man Jing Zi	G250H1505622	61899†	20
PhytoComm	Man Jing Zi	G250H1505622	61900†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Man Jing Zi*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Man Jing Zi	G250H1505122	1
Phytocomm	Man Jing Zi	G250H1505121	1
Phytocomm	Man Jing Zi	G250H1505122	1
PhytoComm	Man Jing Zi	h1505021	1
Phytocomm	Man Jing Zi	H1505922	1
PhytoComm	Man Jing Zi	H150922	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Man Jing Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Man Jing Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	6	2045

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4531 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61899	61899	0.00	62.35
61900	61900	0.00	62.10

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Mo Yao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`50343-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mo Yao; Myrrha resina

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Mo Yao	`G169H0732621`	`61957`	40	from supplier
PhytoComm	Mo Yao	`G169H0732621`	`61958`	40	from supplier
PhytoComm	Mo Yao	`G169H0732621`	`62171`	40	from supplier
PhytoComm	Mo Yao	`G169H0732621`	`62172`	40	from supplier

Validation samples

A total of 23 740 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 *Mo Yao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Mo Yao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mo Yao	G169H0732621	61957†	20
PhytoComm	Mo Yao	G169H0732621	61958†	20
PhytoComm	Mo Yao	G169H0732621	62171†	20
PhytoComm	Mo Yao	G169H0732621	62172†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 8 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Mo Yao*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Mo Yao	G1690732222	1
phytocomm	Mo Yao	G169H0732023	1
Phytocomm	Mo Yao	G169H0732122	2
PhytoComm	Mo Yao	G169H0732222	2
Caelo	Mo Yao	G169H0732222	1
Phytocomm	Mo Yao	H0732922	1

- 2043 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mo Yao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mo Yao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	0	0	8	2043

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4528 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61957	61957	0.00	16.19
61958	61958	0.00	16.53
62171	62171	0.00	15.04
62172	62172	0.00	14.67

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Mu Dan Pi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60113-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mu Dan Pi; Moutan cortex radicis

Special notes

When selecting the *Mu Dan Pi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Mu Dan Pi	`G166H0741621`	`61947`	40	from supplier
PhytoComm	Mu Dan Pi	`G166H0741621`	`61948`	40	from supplier

Validation samples

A total of 23 740 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 *Mu Dan Pi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Mu Dan Pi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mu Dan Pi	G166H0741621	61947†	20
PhytoComm	Mu Dan Pi	G166H0741621	61948†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 8 *Apo-Ident* customers from 6 batches from the substance/substance group *Mu Dan Pi*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Mu Dan Pi	G166H0741421	4
Phytocomm	Mu Dan Pi	G166H0741321	2
PhytoComm	Mu Dan Pi	G166H0741022	1
PhytoComm	Mu Dan Pi	G166H0741121	2
Phytocomm	Mu Dan Pi	G166H0741121	5
Phytocomm	Mu Dan Pi	G166H0741122	3
PhytoComm	Mu Dan Pi	G166H0741122	1
PhytoComm	Mu Dan Pi	G166H0741321	2
Phytocomm	Mu Dan Pi	g166j074122	1

- 2030 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mu Dan Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mu Dan Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	6	0	21	2024

The substance/substance group *Mu Dan Pi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.7637 % (> 99.4897 %)	0.0000 % (≥ 0.0000 %)

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
61947	61947	0.00	8.08
61948	61948	0.00	7.63

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Mu Gua**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60236-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mu Gua; Chaenomelis lagenariae fructus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Mu Gua	G063H0424521	61696	40	from supplier
PhytoComm	Mu Gua	G063H0424621	62085	40	from supplier
PhytoComm	Mu Gua	G063H0424621	62086	40	from supplier

Validation samples

A total of 23 740 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 *Mu Gua*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 120 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 60 spectra from 3 reference samples of the substance/substance group *Mu Gua*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mu Gua	G063H0424521	61696†	20
PhytoComm	Mu Gua	G063H0424621	62085†	20
PhytoComm	Mu Gua	G063H0424621	62086†	20

- 7389 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 8 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Mu Gua*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Mu Gua	G063H0424521	4
PhytoComm	Mu Gua	G063H0424021	2
PhytoComm	Mu Gua	G063H0424221	1
Phytocomm	Mu Gua	G063H0424221	1

- 2043 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mu Gua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mu Gua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 120
Type B	0	60	0	7389
Type C	8	0	8	2035

The substance/substance group *Mu Gua* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.8992 %)	100.0000 % (> 90.0000 %)
Type C	99.6041 % (> 99.3304 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61696	61696	0.00	13.00
62085	62085	0.00	15.96
62086	62086	0.00	16.27

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Niu Bang Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60161-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Niu Bang Zi; Arctii fructus; Arctii lappae fructus

Special notes

When selecting the *Niu Bang Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Niu Bang Zi	`G026H0433521`	`61677`	40	from supplier
PhytoComm	Niu Bang Zi	`G026H0433521`	`61744`	41	from supplier

Validation samples

A total of 23 740 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 81 spectra of 2 reference samples from the substance/substance group *Niu Bang Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 159 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Niu Bang Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Niu Bang Zi	G026H0433521	61677†	20
PhytoComm	Niu Bang Zi	G026H0433521	61744†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 16 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Niu Bang Zi*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Niu Bang Zi	G026H0433321	3
Phytocomm	Niu Bang Zi	G026H0433321	1
phytocomm	Niu Bang Zi	g026h0433321	2
Phytocomm	Niu Bang Zi	G026H0433521	3
Phytocomm	Niu Bang Zi	G026H0433222	2
PhytoComm	Niu Bang Zi	G026H0433222	1
PhytoComm	Niu Bang Zi	H0433021	1
Phytocomm	Niu Bang Zi	H0433021	3

- 2035 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	81	0	14 159
Type B	0	40	0	7409
Type C	0	3	13	2035

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5926 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4522 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61677	61677	0.00	24.05
61744	61744	0.00	22.50

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Nü Zhen Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60065-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nü Zhen Zi; Ligustri lucidi fructus

Special notes

When selecting the *Nü Zhen Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Nü Zhen Zi	G138H0345721	62213	40	from supplier
PhytoComm	Nü Zhen Zi	G138H0345721	62214	40	from supplier

Validation samples

A total of 23 740 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 *Nü Zhen Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Nü Zhen Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Nü Zhen Zi	G138H0345721	62213†	20
PhytoComm	Nü Zhen Zi	G138H0345721	62214†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 7 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Nü Zhen Zi*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Nü Zhen Zi	420319901	2
Phytocomm	Nü Zhen Zi	G138H0345421	1
PhytoComm	Nü Zhen Zi	H0345021	1
PhytoComm	Nü Zhen Zi	G138H0345321	1
PhytoComm	Nü Zhen Zi	420319901	1
PhytoComm	Nü Zhen Zi	h0345021	1

- 2044 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nü Zhen Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nü Zhen Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	0	7	2043

The substance/substance group *Nü Zhen Zi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9627 % (> 99.6891 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62213	62213	0.00	14.58
62214	62214	0.00	14.32

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Pi Pa Ye**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60201-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pi Pa Ye; Eriobotryae japonicae folium

Special notes

When selecting the *Pi Pa Ye* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Pi Pa Ye	`G099H0832521`	`61681`	40	from supplier

Validation samples

A total of 23 740 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 *Pi Pa Ye*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Pi Pa Ye*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Pi Pa Ye	G099H0832521	61681†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Pi Pa Ye*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Pi Pa Ye	G099H0832221	1
Phytocomm	Pi Pa Ye	G099H0832221	1
Herbasinica	Pi Pa Ye	G099H0832221	1
PhytoComm	Pi Pa Ye	H0832922	2

- 2046 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pi Pa Ye* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pi Pa Ye* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	10	0	5	2036

The substance/substance group *Pi Pa Ye* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	99.6101 % (> 99.3368 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61681	61681	0.00	12.31

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Pu Gong Ying**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	50358-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pu Gong Ying; Taraxaci mongolici herba cum radice

Special notes

When selecting the *Pu Gong Ying* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Pu Gong Ying	G239H1315623	62119	40	from supplier
PhytoComm	Pu Gong Ying	G239H1315623	62120	40	from supplier
PhytoComm	Pu Gong Ying	G239H1315623	62163	40	from supplier
PhytoComm	Pu Gong Ying	G239H1315623	62164	40	from supplier

Validation samples

A total of 23 740 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 *Pu Gong Ying*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Pu Gong Ying*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Pu Gong Ying	G239H1315623	62119†	20
PhytoComm	Pu Gong Ying	G239H1315623	62120†	20
PhytoComm	Pu Gong Ying	G239H1315623	62163†	20
PhytoComm	Pu Gong Ying	G239H1315623	62164†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 8 spectra from 5 *Apo-Ident* customers from 2 batches from the substance/substance group *Pu Gong Ying*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Pu Gong Ying	G239H1315321	5
PhytoComm	Pu Gong Ying	G239H1315321	2
PhytoComm	Pu Gong Ying	H1315923	1

- 2043 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pu Gong Ying* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pu Gong Ying* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	3	0	8	2040

The substance/substance group *Pu Gong Ying* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	99.9088 % (> 99.6352 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62119	62119	0.00	14.32
62120	62120	0.00	14.71
62163	62163	0.00	12.38
62164	62164	0.00	12.78

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Qiang Huo**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60109-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Qiang Huo; Notopterygii rhizoma et radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Qiang Huo	G172H0840621	62121	40	from supplier
PhytoComm	Qiang Huo	G172H0840621	62122	40	from supplier

Validation samples

A total of 23 740 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 *Qiang Huo*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Qiang Huo*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Qiang Huo	G172H0840621	62121†	20
PhytoComm	Qiang Huo	G172H0840621	62122†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Qiang Huo*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Qiang Huo	G172H0840321	2
Phytocomm	Qiang Huo	G172H0840321	1
Phytocomm	Qiang Huo	g172h0841321	1
PhytoComm	Qiang Huo	H0840922	2

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Qiang Huo* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Qiang Huo* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14160
Type B	0	40	0	7409
Type C	1	3	3	2044

The substance/substance group *Qiang Huo* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9378 % (> 99.6644 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62121	62121	0.00	9.33
62122	62122	0.00	8.82

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Qin Jiao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60222-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Qin Jiao; Gentianae macrophyllae radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Qin Jiao	G113H1059521	61772	40	from supplier
PhytoComm	Qin Jiao	G113H1059521	61814	40	from supplier

Validation samples

A total of 23 740 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 *Qin Jiao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Qin Jiao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Qin Jiao	G113H1059521	61772†	20
PhytoComm	Qin Jiao	G113H1059521	61814†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 8 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Qin Jiao*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Qin Jiao	G113H1059022	2
PhytoComm	Qin Jiao	G113H1059022	1
Phytocomm	Qin Jiao	G113H1059121	2
PhytoComm	Qin Jiao	G113H1059121	1
PhytoComm	Qin Jiao	G113H1059321	1
PhytoComm	Qin Jiao	H1059922	1

- 2043 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Qin Jiao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Qin Jiao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	8	0	8	2035

The substance/substance group *Qin Jiao* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.6730 % (> 99.3994 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61772	61772	0.00	13.57
61814	61814	0.00	13.87

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Qing Pi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`50371-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Qing Pi; Citri reticulatae viride pericarpium

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Qing Pi	`G074H0809621`	`62041`	40	from supplier
PhytoComm	Qing Pi	`G074H0809621`	`62042`	40	from supplier

Validation samples

A total of 23 740 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 *Qing Pi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Qing Pi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Qing Pi	G074H0809621	62041†	20
PhytoComm	Qing Pi	G074H0809621	62042†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Qing Pi*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Qing Pi	G074H100713	2
Phytocomm	Qing Pi	G074H100713	2
Phytocomm	Qing Pi	g074h100713	1

- 2046 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Qing Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Qing Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	5	2046

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4534 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62041	62041	0.00	9.64
62042	62042	0.00	9.69

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Rou Cong Rong**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60182-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Rou Cong Rong; Cistanchis herba

Special notes

When selecting the *Rou Cong Rong* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Rou Cong Rong	`G072H1460621`	`61834`	40	from supplier

Validation samples

A total of 23 740 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 *Rou Cong Rong*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Rou Cong Rong*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Rou Cong Rong	G072H1460621	61834†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 1 *Apo-Ident* customers from 3 batches from the substance/substance group *Rou Cong Rong*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Rou Cong Rong	G072H1460321	1
PhytoComm	Rou Cong Rong	444151	1
Bios	Rou Cong Rong	434550	1

- 2048 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Rou Cong Rong* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Rou Cong Rong* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	0	0	3	2048

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.4545 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61834	61834	0.00	16.15

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Rou Gui**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60169-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Rou Gui; Cinnamomi cassiae cortex

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Rou Gui	G069HS204QM1	62187	40	from supplier
PhytoComm	Rou Gui	G069HS204QM1	62188	40	from supplier

Validation samples

A total of 23 740 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 *Rou Gui*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 35 spectra from 2 reference samples of the substance/substance group *Rou Gui*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Rou Gui	G069HS204QM1	62187†	15
PhytoComm	Rou Gui	G069HS204QM1	62188†	20

- 7414 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 7 *Apo-Ident* customers from 4 batches from the substance/substance group *Rou Gui*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Rou Gui	G069H0617323	1
Phytocomm	Rou Gui	G069H0617123	1
PhytoComm	Rou Gui	G069H0617323	1
PhytoComm	Rou Gui	G069H0617123	2
Phytocomm	Rou Gui	H0617022	2
Phytocomm	Rou Gui	g069h0617123	1
PhytoComm	Rou Gui	H0617022	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Rou Gui* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Rou Gui* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	34	1	7414
Type C	0	0	9	2042

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8995 %)	97.1429 % (> 88.5714 %)
Type C	100.0000 % (> 99.4526 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62187	62187	0.00	5.42
62188	62188	0.00	4.79

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ru Xiang**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`50370-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ru Xiang; Olibanum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ru Xiang	`G174H0820621`	`61935`	40	from supplier
PhytoComm	Ru Xiang	`G174H0820621`	`61936`	40	from supplier

Validation samples

A total of 23 740 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 *Ru Xiang*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Ru Xiang*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ru Xiang	G174H0820621	61935†	20
PhytoComm	Ru Xiang	G174H0820621	61936†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 7 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Ru Xiang*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Ru Xiang	G174H0820421	1
PhytoComm	Ru Xiang	G174H0820421	2
Phytocomm	Ru Xiang	G174H0820123	1
Phytocomm	Ru Xiang	G174H0820231	1
PhytoComm	Ru Xiang	H0820923	1
PhytoComm	Ru Xiang	G174H0820321	1

- 2044 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ru Xiang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ru Xiang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	7	2044

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4529 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61935	61935	0.00	85.97
61936	61936	0.00	83.52

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**San Leng**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60029-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

San Leng; Sparganii rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	San Leng	G270H0311721	62235	40	from supplier
PhytoComm	San Leng	G270H0311721	62236	40	from supplier

Validation samples

A total of 23 740 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 *San Leng*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *San Leng*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	San Leng	G270H0311721	62235†	20
PhytoComm	San Leng	G270H0311721	62236†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 4 batches from the substance/substance group *San Leng*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	San Leng	G270H0311121	1
Phytocomm	San Leng	g270h0311221	1
PhytoComm	San Leng	G270H0311221	1
Phytocomm	San Leng	H0311922	1

- 2047 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *San Leng* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *San Leng* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	11	1	3	2036

The substance/substance group *San Leng* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.6274 % (> 99.3543 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62235	62235	0.00	12.76
62236	62236	0.00	13.46

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**San Qi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60415-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

San Qi; Notoginseng radix; Pseudoginseng radix

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	San Qi	G203H0312621	62135	40	from supplier
PhytoComm	San Qi	G203H0312621	62136	40	from supplier
PhytoComm	San Qi	G203H0312721	62245	40	from supplier
PhytoComm	San Qi	G203H0312721	62246	40	from supplier

Validation samples

A total of 23 740 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 *San Qi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *San Qi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	San Qi	G203H0312621	62135†	20
PhytoComm	San Qi	G203H0312621	62136†	20
PhytoComm	San Qi	G203H0312721	62245†	20
PhytoComm	San Qi	G203H0312721	62246†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 4 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *San Qi*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phytocomm	San Qi	G203H0312021	1
PhytoComm	San Qi	G203H0312021	2
Phytocomm	San Qi	g203h0312021	1

- 2047 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *San Qi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *San Qi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	1	0	4	2046

The substance/substance group *San Qi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	99.9067 % (> 99.6336 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62135	62135	0.00	11.58
62136	62136	0.00	11.25
62245	62245	0.00	11.75
62246	62246	0.00	11.74

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Sang Bai Pi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	50287-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sang Bai Pi; Mori cortex

Special notes

When selecting the *Sang Bai Pi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Sang Bai Pi	G161H1042721	62253	40	from supplier
PhytoComm	Sang Bai Pi	G161H1042721	62254	40	from supplier

Validation samples

A total of 23 740 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 *Sang Bai Pi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Sang Bai Pi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sang Bai Pi	G161H1042721	62253†	20
PhytoComm	Sang Bai Pi	G161H1042721	62254†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Sang Bai Pi*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Sang Bai Pi	G161H1042321	3
PhytoComm	Sang Bai Pi	G161H1042322	1
PhytoComm	Sang Bai Pi	G161H1042121	2
Phytocomm	Sang Bai Pi	G161H1042321	1
Phytocomm	Sang Bai Pi	G161H1042922	1
PhytoComm	Sang Bai Pi	G161H1042922	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sang Bai Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sang Bai Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	2	0	9	2040

The substance/substance group *Sang Bai Pi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.8534 % (> 99.5797 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62253	62253	0.00	12.95
62254	62254	0.00	12.92

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Sang Ye**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60079-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sang Ye; Mori albi folium

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Sang Ye	G162H1043621	61973	40	from supplier
PhytoComm	Sang Ye	G162H1043621	61974	40	from supplier

Validation samples

A total of 23 740 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 *Sang Ye*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Sang Ye*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sang Ye	G162H1043621	61973†	20
PhytoComm	Sang Ye	G162H1043621	61974†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Sang Ye*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Sang Ye	421013801	1
Phytocomm	Sang Ye	G162H1043421	3
PhytoComm	Sang Ye	G162H1043121	1
Phytocomm	Sang Ye	G162H1043121	4
PhytoComm	Sang Ye	H1043021	1

- 2041 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sang Ye* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sang Ye* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	10	2041

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61973	61973	0.00	13.67
61974	61974	0.00	13.69

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Sang Zhi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60091-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sang Zhi; Mori albae ramulus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Sang Zhi	`G164H1044621`	`61969`	40	from supplier
PhytoComm	Sang Zhi	`G164H1044621`	`61970`	40	from supplier

Validation samples

A total of 23 740 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 *Sang Zhi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Sang Zhi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sang Zhi	G164H1044621	61969†	20
PhytoComm	Sang Zhi	G164H1044621	61970†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Sang Zhi*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Sang Zhi	G164H1044022	4
PhytoComm	Sang Zhi	G164H1044022	1
PhytoComm	Sang Zhi	G164H1044221	1
Phytocomm	Sang Zhi	G164H1044221	1
PhytoComm	Sang Zhi	H1044921	2

- 2042 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sang Zhi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sang Zhi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	3	0	9	2039

The substance/substance group *Sang Zhi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9067 % (> 99.6330 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61969	61969	0.00	8.74
61970	61970	0.00	8.60

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Sha Ren**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60184-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sha Ren; Amomi villosi fructus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Sha Ren	G018H0939522	61703	40	from supplier
PhytoComm	Sha Ren	G018H0939523	61799	40	from supplier
PhytoComm	Sha Ren	G018H0939523	61818	40	from supplier
PhytoComm	Sha Ren	G018H0939622	62095	40	from supplier
PhytoComm	Sha Ren	G018H0939622	62096	40	from supplier

Validation samples

A total of 23 740 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 *Sha Ren*. These samples are listed above in the section *calibration samples*. The reference samples originate from 3 different batches.

- 14 040 spectra from a total of 175 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 100 spectra from 5 reference samples of the substance/substance group *Sha Ren*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sha Ren	G018H0939522	61703†	20
PhytoComm	Sha Ren	G018H0939523	61799†	20
PhytoComm	Sha Ren	G018H0939523	61818†	20
PhytoComm	Sha Ren	G018H0939622	62095†	20
PhytoComm	Sha Ren	G018H0939622	62096†	20

- 7349 spectra from a total of 178 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 12 spectra from 8 *Apo-Ident* customers from 5 batches from the substance/substance group *Sha Ren*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Sha Ren	G018H0939523	1
PhytoComm	Sha Ren	G018H0939321	1
Phytocomm	Sha Ren	G018H0939522	1
Phytocomm	Sha Ren	G018H0939321	1
Phytocomm	Sha Ren	g018h0939321	1
PhytoComm	Sha Ren	H0939022	4
Phytocomm	Sha Ren	H0939022	2
Euro OTC	Sha Ren	H0939022	1

- 2039 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sha Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sha Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14040
Type B	0	100	0	7349
Type C	5	4	8	2034

The substance/substance group *Sha Ren* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9477 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 94.0000 %)
Type C	99.6891 % (> 99.4153 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61703	61703	0.00	10.80
61799	61799	0.00	15.94
61818	61818	0.00	17.05
62095	62095	0.00	16.07
62096	62096	0.00	14.66

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Shan Yu Rou**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60226-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Shan Yu Rou; Corni officinalis fructus

Special notes

When selecting the *Shan Yu Rou* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Shan Yu Rou	G080H0333621	62011	40	from supplier
PhytoComm	Shan Yu Rou	G080H0333621	62012	40	from supplier

Validation samples

A total of 23 740 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 *Shan Yu Rou*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Shan Yu Rou*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Shan Yu Rou	G080H0333621	62011†	20
PhytoComm	Shan Yu Rou	G080H0333621	62012†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Shan Yu Rou*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Shan Yu Rou	G080H0333421	1
PhytoComm	Shan Yu Rou	G080H0333021	2
Phytocomm	Shan Yu Rou	G080H0333021	1
Phytocomm	Shan Yu Rou	G080H0333121	2
PhytoComm	Shan Yu Rou	G080H033321	1
Phytocomm	Shan Yu Rou	G080H0333221	1
Phytocomm	Shan Yu Rou	g080h0333221	1
PhytoComm	Shan Yu Rou	G080H0333121	1

- 2041 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Shan Yu Rou* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Shan Yu Rou* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	5	0	10	2036

The substance/substance group *Shan Yu Rou* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.5750 % (> 99.3013 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62011	62011	0.00	18.01
62012	62012	0.00	18.23

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Shan Zha**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60192-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Shan Zha; Crataegi fructus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Shan Zha	G082H0331522	62029	40	from supplier
PhytoComm	Shan Zha	G082H0331522	62030	40	from supplier

Validation samples

A total of 23 740 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 *Shan Zha*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Shan Zha*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Shan Zha	G082H0331522	62029†	20
PhytoComm	Shan Zha	G082H0331522	62030†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 9 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Shan Zha*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Shan Zha	G082H0331521	1
phytocomm	Shan Zha	G082H0331022	1
PhytoComm	Shan Zha	G082H0331022	4
Phytocomm	Shan Zha	G082H0331022	1
PhytoComm	Shan Zha	G082H0331324	1
Phytocomm	Shan Zha	G082H0331324	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Shan Zha* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Shan Zha* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	0	9	2041

The substance/substance group *Shan Zha* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9733 % (> 99.6997 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62029	62029	0.00	11.06
62030	62030	0.00	10.00

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**She Gan**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60335-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

She Gan; Belamcandae rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	She Gan	G048H1034621	61771	40	from supplier
PhytoComm	She Gan	G048H1034621	61828	40	from supplier

Validation samples

A total of 23 740 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 *She Gan*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *She Gan*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	She Gan	G048H1034621	61771†	20
PhytoComm	She Gan	G048H1034621	61828†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 3 batches from the substance/substance group *She Gan*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	She Gan	G048H1034422	1
PhytoComm	She Gan	G048H1034021	1
Phytocomm	She Gan	G048H1034021	2
Phytocomm	She Gan	G048H1034122	2

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *She Gan* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *She Gan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	8	1	5	2037

The substance/substance group *She Gan* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.8290 % (> 99.5555 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61771	61771	0.00	8.52
61828	61828	0.00	9.24

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Shen Qu**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60020-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Shen Qu; Massa fermentata medicinalis

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Shen Qu	G156H0935521	61665	40	from supplier
PhytoComm	Shen Qu	G156H0935522	61971	40	from supplier
PhytoComm	Shen Qu	G156H0935522	61972	40	from supplier
PhytoComm	Shen Qu	G156H0935621	62259	40	from supplier
PhytoComm	Shen Qu	G156H0935621	62260	40	from supplier

Validation samples

A total of 23 740 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 *Shen Qu*. These samples are listed above in the section *calibration samples*. The reference samples originate from 3 different batches.

- 14 040 spectra from a total of 175 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 100 spectra from 5 reference samples of the substance/substance group *Shen Qu*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Shen Qu	G156H0935521	61665†	20
PhytoComm	Shen Qu	G156H0935522	61971†	20
PhytoComm	Shen Qu	G156H0935522	61972†	20
PhytoComm	Shen Qu	G156H0935621	62259†	20
PhytoComm	Shen Qu	G156H0935621	62260†	20

- 7349 spectra from a total of 178 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 9 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Shen Qu*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Shen Qu	G156H0935521	1
PhytoComm	Shen Qu	G156H0935521	1
phytocomm	Shen Qu	G156H0935023	1
Phytocomm	Shen Qu	G156H0935023	1
PhytoComm	Shen Qu	G156H0935121	2
phytocomm	Shen Qu	g156h0935421	1
PhytoComm	Shen Qu	H0935021	2

- 2042 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Shen Qu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Shen Qu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 040
Type B	0	100	0	7349
Type C	0	2	7	2042

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9477 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.4526 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61665	61665	0.00	23.18
61971	61971	0.00	25.34
61972	61972	0.00	25.71
62259	62259	0.00	27.07
62260	62260	0.00	26.89

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Sheng Jiang**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60017-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sheng Jiang; Zingiberis rhizoma recens

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Sheng Jiang	G253H0534522	61650	40	from supplier
PhytoComm	Sheng Jiang	G253H0534623	62141	40	from supplier
PhytoComm	Sheng Jiang	G253H0534623	62142	40	from supplier

Validation samples

A total of 23 740 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 *Sheng Jiang*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 120 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 60 spectra from 3 reference samples of the substance/substance group *Sheng Jiang*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sheng Jiang	G253H0534522	61650†	20
PhytoComm	Sheng Jiang	G253H0534623	62141†	20
PhytoComm	Sheng Jiang	G253H0534623	62142†	20

- 7389 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 11 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Sheng Jiang*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Sheng Jiang	G253H0534522	1
PhytoComm	Sheng Jiang	G253H0534522	3
PhytoComm	Sheng Jiang	G253H0534221	1
Phytocomm	Sheng Jiang	G253H0534221	2
PhytoComm	Sheng Jiang	G253H0534321	2
PhytoComm	Sheng Jiang	H0534022	1
Phytocomm	Sheng Jiang	H0534022	1

- 2040 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sheng Jiang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sheng Jiang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 120
Type B	4	60	0	7385
Type C	4	3	8	2036

The substance/substance group *Sheng Jiang* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 95.0000 %)
Type B	99.9695 % (> 99.9191 %)	100.0000 % (> 90.0000 %)
Type C	99.8299 % (> 99.5561 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61650	61650	0.00	11.88
62141	62141	0.00	7.98
62142	62142	0.00	9.02

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Sheng Ma**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60216-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sheng Ma; Cimicifugae rhizoma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Sheng Ma	G068H0437621	62079	40	from supplier
PhytoComm	Sheng Ma	G068H0437621	62080	40	from supplier

Validation samples

A total of 23 740 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 *Sheng Ma*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Sheng Ma*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sheng Ma	G068H0437621	62079†	20
PhytoComm	Sheng Ma	G068H0437621	62080†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 7 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Sheng Ma*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Sheng Ma	G068H0437421	2
Phytocomm	Sheng Ma	g068h04317121	1
PhytoComm	Sheng Ma	G068H0437021	1
Phytocomm	Sheng Ma	G068H0437121	1
PhytoComm	Sheng Ma	G068H0437121	2

- 2044 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sheng Ma* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sheng Ma* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	7	2044

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4529 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62079	62079	0.00	10.54
62080	62080	0.00	10.47

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Shu Di (Huang)**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60006-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Shu Di (Huang); Rehmanniae praeparata radix; Rehmanniae radix praep.

Special notes

When selecting the *Shu Di (Huang)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Shu Di (Huang)	G210H1601721	62249	40	from supplier
PhytoComm	Shu Di (Huang)	G210H1601721	62250	40	from supplier

Validation samples

A total of 23 740 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 *Shu Di (Huang)*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Shu Di (Huang)*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Shu Di (Huang)	G210H1601721	62249†	20
PhytoComm	Shu Di (Huang)	G210H1601721	62250†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

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

- 19 spectra from 9 *Apo-Ident* customers from 6 batches from the substance/substance group *Shu Di (Huang)*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Shu Di (Huang)	G210H1601421	5
Phytocomm	Shu Di (Huang)	G210H1601521	3
Phytocomm	Shu Di (Huang)	G210H1601221	1
PhytoComm	Shu Di (Huang)	G210H1601121	3
PhytoComm	Shu Di (Huang)	G210H1601221	1
Phytocomm	Shu Di (Huang)	g210h1601221	4
Phytocomm	Shu Di (Huang)	G210H1601121	1
PhytoComm	Shu Di (Huang)	H1601021	1

- 2032 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Shu Di (Huang)* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Shu Di (Huang)* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	5	14	2032

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4522 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62249	62249	0.00	7.51
62250	62250	0.00	8.02

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Suan Zao Ren**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60059-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Suan Zao Ren; Zizyphi spinosae semen

Special notes

When selecting the *Suan Zao Ren* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Suan Zao Ren	G254H1418621	61893	40	from supplier
PhytoComm	Suan Zao Ren	G254H1418621	61894	40	from supplier
PhytoComm	Suan Zao Ren	G254H1418622	62133	40	from supplier
PhytoComm	Suan Zao Ren	G254H1418622	62134	40	from supplier

Validation samples

A total of 23 740 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 *Suan Zao Ren*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Suan Zao Ren*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Suan Zao Ren	G254H1418621	61893†	20
PhytoComm	Suan Zao Ren	G254H1418621	61894†	20
PhytoComm	Suan Zao Ren	G254H1418622	62133†	20
PhytoComm	Suan Zao Ren	G254H1418622	62134†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 6 spectra from 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Suan Zao Ren*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Suan Zao Ren	G254H1418421	1
Phytocomm	Suan Zao Ren	G254H1418121	2
PhytoComm	Suan Zao Ren	G254H1418121	1
Phytocomm	Suan Zao Ren	g254h1418121	2

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Suan Zao Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Suan Zao Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	0	0	6	2045

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4531 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61893	61893	0.00	18.67
61894	61894	0.00	19.88
62133	62133	0.00	27.46
62134	62134	0.00	27.76

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Tao Ren**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60454-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tao Ren; Persicae semen

Special notes

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

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

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

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

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

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tao Ren*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Tao Ren	`G184H1007621`	`61943`	40	from supplier
PhytoComm	Tao Ren	`G184H1007621`	`61944`	40	from supplier

Validation samples

A total of 23 740 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 *Tao Ren*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Tao Ren*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Tao Ren	G184H1007621	61943†	20
PhytoComm	Tao Ren	G184H1007621	61944†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 8 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Tao Ren*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phytocomm	Tao Ren	G184H1007023	1
phytocomm	Tao Ren	G184H1007122	2
PhytoComm	Tao Ren	G184H1007122	2
Phytocomm	Tao Ren	g184h1007122	1
PhytoComm	Tao Ren	G184H1007321	2

- 2043 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tao Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tao Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	8	2043

The substance/substance group *Tao Ren* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4528 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61943	61943	0.00	45.20
61944	61944	0.00	45.85

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Tu Fu Ling**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`50885-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tu Fu Ling; Smilacis glabrae rhizoma

Special notes

When selecting the *Tu Fu Ling* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tu Fu Ling*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Tu Fu Ling	`G231H0325621`	`61915`	40	from supplier
PhytoComm	Tu Fu Ling	`G231H0325621`	`61916`	40	from supplier

Validation samples

A total of 23 740 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 *Tu Fu Ling*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Tu Fu Ling*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Tu Fu Ling	G231H0325621	61915†	20
PhytoComm	Tu Fu Ling	G231H0325621	61916†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 11 spectra from 7 *Apo-Ident* customers from 4 batches from the substance/substance group *Tu Fu Ling*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Tu Fu Ling	G231H0325121	5
PhytoComm	Tu Fu Ling	G231H0325121	1
Phytocomm	Tu Fu Ling	G231H0325421	2
PhytoComm	Tu Fu Ling	G231H0325421	1
Phytocomm	Tu Fu Ling	G231H325121	1
PhytoComm	Tu Fu Ling	G23H0325121	1

- 2040 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tu Fu Ling* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tu Fu Ling* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	1	10	2040

The substance/substance group *Tu Fu Ling* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61915	61915	0.00	12.06
61916	61916	0.00	12.34

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Tu Si Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60217-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tu Si Zi; Cuscutae semen

Special notes

When selecting the *Tu Si Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tu Si Zi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Tu Si Zi	`G086H1243521`	`61680`	40	from supplier

Validation samples

A total of 23 740 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 *Tu Si Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Tu Si Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Tu Si Zi	G086H1243521	61680†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 9 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Tu Si Zi*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Tu Si Zi	G086H1243521	3
PhytoComm	Tu Si Zi	G086H1243521	1
Phytocomm	Tu Si Zi	161213tsz	1
Phytocomm	Tu Si Zi	H1243022	1
PhytoComm	Tu Si Zi	H1243022	1
Phytocomm	Tu Si Zi	h1243022	1
Phytocomm	Tu Si Zi	H1243923	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tu Si Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tu Si Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	0	4	5	2042

The substance/substance group *Tu Si Zi* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.4526 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61680	61680	0.00	26.02

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Wang Bu Liu Xing**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	50390-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wang Bu Liu Xing; Vaccariae semen

Special notes

When selecting the *Wang Bu Liu Xing* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Wang Bu Liu Xing*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Wang Bu Liu Xing	G281HS057QM1	62181	40	from supplier
PhytoComm	Wang Bu Liu Xing	G281HS057QM1	62182	40	from supplier

Validation samples

A total of 23 740 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 *Wang Bu Liu Xing*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Wang Bu Liu Xing*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wang Bu Liu Xing	G281HS057QM1	62181†	20
PhytoComm	Wang Bu Liu Xing	G281HS057QM1	62182†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 8 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Wang Bu Liu Xing*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Wang Bu Liu Xing	G281H0456221	1
PhytoComm	Wang Bu Liu Xing	G281H0456322	1
Phytocomm	Wang Bu Liu Xing	G281H0456521	1
PhytoComm	Wang Bu Liu Xing	G281H456421	1
Phytocomm	Wang Bu Liu Xing	G281H0456221	2
PhytoComm	Wang Bu Liu Xing	H0456021	1
Phytocomm	Wang Bu Liu Xing	H0456021	1

- 2043 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Wang Bu Liu Xing* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wang Bu Liu Xing* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	3	40	0	7406
Type C	0	0	8	2043

The substance/substance group *Wang Bu Liu Xing* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	99.9479 % (> 99.8976 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4528 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62181	62181	0.00	6.07
62182	62182	0.00	5.28

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Wei Ling Xian**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60543-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wei Ling Xian; Clematidis radix

Special notes

When selecting the *Wei Ling Xian* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Wei Ling Xian*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Wei Ling Xian	G075H0943521	62031	40	from supplier
PhytoComm	Wei Ling Xian	G075H0943521	62032	40	from supplier

Validation samples

A total of 23 740 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 *Wei Ling Xian*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Wei Ling Xian*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wei Ling Xian	G075H0943521	62031†	20
PhytoComm	Wei Ling Xian	G075H0943521	62032†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 11 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Wei Ling Xian*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Wei Ling Xian	G075H0943223	2
PhytoComm	Wei Ling Xian	G075H0943223	4
Phytocomm	Wei Ling Xian	g075h0943223	1
Phytocomm	Wei Ling Xian	G075H0943422	1
PhytoComm	Wei Ling Xian	420905402	2
PhytoComm	Wei Ling Xian	G075H0943223	1

- 2040 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Wei Ling Xian* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wei Ling Xian* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	11	2040

The substance/substance group *Wei Ling Xian* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62031	62031	0.00	10.63
62032	62032	0.00	10.27

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Wu Jia Pi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60149-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wu Jia Pi; Acanthopanacis cortex; Acanthopanacis cortex radicis

Special notes

When selecting the *Wu Jia Pi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Wu Jia Pi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Wu Jia Pi	G002H0402621	62047	40	from supplier
PhytoComm	Wu Jia Pi	G002H0402621	62048	40	from supplier
PhytoComm	Wu Jia Pi	G002H0402621	62151	40	from supplier
PhytoComm	Wu Jia Pi	G002H0402621	62152	40	from supplier

Validation samples

A total of 23 740 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 *Wu Jia Pi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Wu Jia Pi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wu Jia Pi	G002H0402621	62047†	20
PhytoComm	Wu Jia Pi	G002H0402621	62048†	20
PhytoComm	Wu Jia Pi	G002H0402621	62151†	20
PhytoComm	Wu Jia Pi	G002H0402621	62152†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 8 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Wu Jia Pi*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Wu Jia Pi	G002H0402321	3
Phytocomm	Wu Jia Pi	G002H0402321	2
Phytocomm	Wu Jia Pi	g002h0402321	1
PhytoComm	Wu Jia Pi	H0402021	1
Phytocomm	Wu Jia Pi	H042021	1

- 2043 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Wu Jia Pi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wu Jia Pi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	0	0	8	2043

The substance/substance group *Wu Jia Pi* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4528 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62047	62047	0.00	16.41
62048	62048	0.00	16.29
62151	62151	0.00	16.92
62152	62152	0.00	17.09

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Wu Wei Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60001-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wu Wei Zi; Schisandrae chinensis fructus

Special notes

When selecting the *Wu Wei Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Wu Wei Zi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Wu Wei Zi	G220H0401621	61925	40	from supplier
PhytoComm	Wu Wei Zi	G220H0401621	61926	40	from supplier

Validation samples

A total of 23 740 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 *Wu Wei Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Wu Wei Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wu Wei Zi	G220H0401621	61925†	20
PhytoComm	Wu Wei Zi	G220H0401621	61926†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 8 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Wu Wei Zi*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phytocomm	Wu Wei Zi	H0401021	1
Phytocomm	Wu Wei Zi	G220H0401421	2
PhytoComm	Wu Wei Zi	G220H0401122	1
Phytocomm	Wu Wei Zi	H0401021	2
PhytoComm	Wu Wei Zi	H0401021	2

- 2043 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Wu Wei Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wu Wei Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	8	2043

The substance/substance group *Wu Wei Zi* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4528 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61925	61925	0.00	50.26
61926	61926	0.00	50.88

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Wu Yao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60040-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wu Yao; Linderae radix

Special notes

When selecting the *Wu Yao* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Wu Yao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Wu Yao	G140H1025721	62233	40	from supplier
PhytoComm	Wu Yao	G140H1025721	62234	40	from supplier

Validation samples

A total of 23 740 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 *Wu Yao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Wu Yao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wu Yao	G140H1025721	62233†	20
PhytoComm	Wu Yao	G140H1025721	62234†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 7 *Apo-Ident* customers from 4 batches from the substance/substance group *Wu Yao*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Wu Yao	G140H1025521	2
PhytoComm	Wu Yao	G140H1025521	1
PhytoComm	Wu Yao	G140H1025221	2
Phytocomm	Wu Yao	g140h1025221	1
phytocomm	Wu Yao	H1025021	1
PhytoComm	Wu Yao	H1025021	3

- 2041 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Wu Yao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wu Yao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	10	3	7	2031

The substance/substance group *Wu Yao* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.5621 % (> 99.2884 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62233	62233	0.00	8.11
62234	62234	0.00	9.01

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Xi Yang Shen**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60422-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xi Yang Shen; Panacis quinquefolii radix

Special notes

When selecting the *Xi Yang Shen* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xi Yang Shen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xi Yang Shen	G324HS407PP1	61863	40	from supplier
PhytoComm	Xi Yang Shen	G324HS407PP1	61864	40	from supplier

Validation samples

A total of 23 740 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 *Xi Yang Shen*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Xi Yang Shen*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xi Yang Shen	G324HS407PP1	61863†	20
PhytoComm	Xi Yang Shen	G324HS407PP1	61864†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Xi Yang Shen*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Xi Yang Shen	G324HS407OL1	1
Phytocomm	Xi Yang Shen	G324H0647021	2
PhytoComm	Xi Yang Shen	G324H0647321	1
Phytocomm	Xi Yang Shen	G324H0647321	1
Phytocomm	Xi Yang Shen	g324h0647321	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xi Yang Shen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xi Yang Shen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	6	2045

The substance/substance group *Xi Yang Shen* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4531 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61863	61863	0.00	21.75
61864	61864	0.00	21.60

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Xia Ku Cao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60080-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xia Ku Cao; Prunellae vulgaris spica

Special notes

When selecting the *Xia Ku Cao* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xia Ku Cao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xia Ku Cao	G202HS232QM1	62191	40	from supplier
PhytoComm	Xia Ku Cao	G202HS232QM1	62192	40	from supplier

Validation samples

A total of 23 740 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 *Xia Ku Cao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Xia Ku Cao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xia Ku Cao	G202HS232QM1	62191†	20
PhytoComm	Xia Ku Cao	G202HS232QM1	62192†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 11 spectra from 8 *Apo-Ident* customers from 6 batches from the substance/substance group *Xia Ku Cao*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Xia Ku Cao	G202H1064022	1
PhytoComm	Xia Ku Cao	G202H1064121	1
Phytocomm	Xia Ku Cao	g202h1064121	1
Phytocomm	Xia Ku Cao	G202H1064221	3
PhytoComm	Xia Ku Cao	G202H1064221	3
Phytocomm	Xia Ku Cao	G202H1064421	1
Phytocomm	Xia Ku Cao	H1064922	1

- 2040 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xia Ku Cao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xia Ku Cao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	11	2040

The substance/substance group *Xia Ku Cao* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62191	62191	0.00	20.15
62192	62192	0.00	20.15

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Xiao Hui Xiang**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60209-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xiao Hui Xiang; Foeniculi vulgaris fructus

Special notes

When selecting the *Xiao Hui Xiang* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xiao Hui Xiang*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xiao Hui Xiang	G104H0339622	61987	40	from supplier
PhytoComm	Xiao Hui Xiang	G104H0339622	61988	40	from supplier

Validation samples

A total of 23 740 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 *Xiao Hui Xiang*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Xiao Hui Xiang*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xiao Hui Xiang	G104H0339622	61987†	20
PhytoComm	Xiao Hui Xiang	G104H0339622	61988†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 7 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Xiao Hui Xiang*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Xiao Hui Xiang	g104h0339321	1
Phytocomm	Xiao Hui Xiang	G104H0339522	3
PhytoComm	Xiao Hui Xiang	G104H0339321	1
PhytoComm	Xiao Hui Xiang	H0339021	2

- 2044 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xiao Hui Xiang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xiao Hui Xiang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	3	4	2043

The substance/substance group *Xiao Hui Xiang* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9661 % (> 99.6925 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61987	61987	0.00	15.98
61988	61988	0.00	15.52

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Xie Bai**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60362-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xie Bai; Allii bulbus; Allii macrostemonis bulbus

Special notes

When selecting the *Xie Bai* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xie Bai*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xie Bai	G504H1830621	62109	40	from supplier
PhytoComm	Xie Bai	G504H1830621	62110	40	from supplier

Validation samples

A total of 23 740 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 *Xie Bai*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Xie Bai*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xie Bai	G504H1830621	62109†	20
PhytoComm	Xie Bai	G504H1830621	62110†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 *Xie Bai*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Xie Bai	G504H1830421	1
Phytocomm	Xie Bai	G504H1830422	1
PhytoComm	Xie Bai	G504H1830121	1
PhytoComm	Xie Bai	G504H1830321	1

- 2047 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xie Bai* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xie Bai* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	4	2047

The substance/substance group *Xie Bai* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4538 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62109	62109	0.00	15.34
62110	62110	0.00	15.74

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Xin Yi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60231-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xin Yi; Magnoliae flos

Special notes

When selecting the *Xin Yi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xin Yi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xin Yi	G153H0758721	62255	40	from supplier
PhytoComm	Xin Yi	G153H0758721	62256	40	from supplier

Validation samples

A total of 23 740 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 *Xin Yi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Xin Yi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xin Yi	G153H0758721	62255†	20
PhytoComm	Xin Yi	G153H0758721	62256†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Xin Yi*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Xin Yi	`161213xy`	1
Phytocomm	Xin Yi	`G153H0758521`	1
PhytoComm	Xin Yi	`G153H0758121`	3
Phytocomm	Xin Yi	`G153H0758121`	3
PhytoComm	Xin Yi	`G153H0758321`	2

- 2041 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xin Yi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xin Yi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	10	2041

The substance/substance group *Xin Yi* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62255	62255	0.00	26.05
62256	62256	0.00	25.71

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Xu Duan**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60245-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xu Duan; Dipsaci radix

Special notes

When selecting the *Xu Duan* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xu Duan*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xu Duan	G092H2106621	62007	40	from supplier
PhytoComm	Xu Duan	G092H2106621	62008	40	from supplier

Validation samples

A total of 23 740 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 *Xu Duan*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Xu Duan*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xu Duan	G092H2106621	62007†	20
PhytoComm	Xu Duan	G092H2106621	62008†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Xu Duan*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Xu Duan	G092H2106422	1
PhytoComm	Xu Duan	G092H2106023	2
PhytoComm	Xu Duan	G092H2106321	1

- 2047 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xu Duan* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xu Duan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	2	0	4	2045

The substance/substance group *Xu Duan* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9005 % (> 99.6274 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62007	62007	0.00	14.38
62008	62008	0.00	14.56

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Xuan Fu Hua**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60223-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xuan Fu Hua; Inulae flos

Special notes

When selecting the *Xuan Fu Hua* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xuan Fu Hua*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xuan Fu Hua	`G126H1168521`	`61664`	40	from supplier

Validation samples

A total of 23 740 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 *Xuan Fu Hua*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Xuan Fu Hua*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xuan Fu Hua	G126H1168521	61664†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Xuan Fu Hua*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Xuan Fu Hua	G126H1168521	1
PhytoComm	Xuan Fu Hua	G126H1168121	1
Phytocomm	Xuan Fu Hua	G126H1168121	1
PhytoComm	Xuan Fu Hua	H1168921	2
Phytocomm	Xuan Fu Hua	H1168921	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xuan Fu Hua* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xuan Fu Hua* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	0	1	5	2045

The substance/substance group *Xuan Fu Hua* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.4531 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61664	61664	0.00	13.26

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Xuan Shen**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60095-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xuan Shen; Scrophulariae ningpoensis radix

Special notes

When selecting the *Xuan Shen* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xuan Shen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xuan Shen	G223HS092QH1	62199	40	from supplier
PhytoComm	Xuan Shen	G223HS092QH1	62200	40	from supplier
PhytoComm	Xuan Shen	G223H0537521	62205	40	from supplier
PhytoComm	Xuan Shen	G223H0537521	62206	40	from supplier

Validation samples

A total of 23 740 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 *Xuan Shen*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Xuan Shen*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xuan Shen	G223HS092QH1	62199†	20
PhytoComm	Xuan Shen	G223HS092QH1	62200†	20
PhytoComm	Xuan Shen	G223H0537521	62205†	20
PhytoComm	Xuan Shen	G223H0537521	62206†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 12 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Xuan Shen*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Xuan Shen	G223H0537421	1
PhytoComm	Xuan Shen	G223H0537221	3
Phytocomm	Xuan Shen	G223H0537221	1
Phytocomm	Xuan Shen	g22h0537322	1
PhytoComm	Xuan Shen	G223H0537322	1
Phytocomm	Xuan Shen	H0537021	2
Euro OTC	Xuan Shen	H0537021	1
PhytoComm	Xuan Shen	H0537021	2

- 2039 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xuan Shen* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xuan Shen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	6	4	8	2033

The substance/substance group *Xuan Shen* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	99.8603 % (> 99.5866 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62199	62199	0.00	8.67
62200	62200	0.00	9.14
62205	62205	0.00	11.46
62206	62206	0.00	11.95

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Yan Hu Suo**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60439-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Yan Hu Suo; Corydalis rhizoma

Special notes

When selecting the *Yan Hu Suo* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Yan Hu Suo*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yan Hu Suo	G081H0805622	62039	40	from supplier
PhytoComm	Yan Hu Suo	G081H0805622	62040	40	from supplier

Validation samples

A total of 23 740 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 *Yan Hu Suo*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Yan Hu Suo*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yan Hu Suo	G081H0805622	62039†	20
PhytoComm	Yan Hu Suo	G081H0805622	62040†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 9 *Apo-Ident* customers from 6 batches from the substance/substance group *Yan Hu Suo*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Yan Hu Suo	G081F1000301	3
Phytocomm	Yan Hu Suo	G081F1000301	1
Phytocomm	Yan Hu Suo	g081f1000301	1
Phytocomm	Yan Hu Suo	G081H0805221	1
PhytoComm	Yan Hu Suo	G081H0805221	1
PhytoComm	Yan Hu Suo	G081H0805223	1
Phytocomm	Yan Hu Suo	G081H0805223	1
Phytocomm	Yan Hu Suo	G081H0805521	1
PhytoComm	Yan Hu Suo	G081H0805521	1
PhytoComm	Yan Hu Suo	G081H0805223	1

- 2039 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Yan Hu Suo* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yan Hu Suo* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	2	1	11	2037

The substance/substance group *Yan Hu Suo* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9128 % (> 99.6390 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62039	62039	0.00	6.58
62040	62040	0.00	6.50

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ye Jiao Teng**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60068-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ye Jiao Teng; Polygoni multiflori caulis

Special notes

When selecting the *Ye Jiao Teng* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ye Jiao Teng*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ye Jiao Teng	G288H0885522	61750	40	from supplier
PhytoComm	Ye Jiao Teng	G288H0885522	62051	40	from supplier
PhytoComm	Ye Jiao Teng	G288H0885522	62052	40	from supplier
PhytoComm	Ye Jiao Teng	G288H0885621	62131	40	from supplier
PhytoComm	Ye Jiao Teng	G288H0885621	62132	40	from supplier

Validation samples

A total of 23 740 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 *Ye Jiao Teng*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 040 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 100 spectra from 5 reference samples of the substance/substance group *Ye Jiao Teng*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ye Jiao Teng	G288H0885522	61750†	20
PhytoComm	Ye Jiao Teng	G288H0885522	62051†	20
PhytoComm	Ye Jiao Teng	G288H0885522	62052†	20
PhytoComm	Ye Jiao Teng	G288H0885621	62131†	20
PhytoComm	Ye Jiao Teng	G288H0885621	62132†	20

- 7349 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 9 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Ye Jiao Teng*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Ye Jiao Teng	G288H0885223	2
Phytocomm	Ye Jiao Teng	G288H0885522	2
PhytoComm	Ye Jiao Teng	G288H0885522	2
Phytocomm	Ye Jiao Teng	g228h0085223	1
PhytoComm	Ye Jiao Teng	H0885021	1
Phytocomm	Ye Jiao Teng	H0885922	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ye Jiao Teng* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ye Jiao Teng* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14040
Type B	0	100	0	7349
Type C	0	4	5	2042

The substance/substance group *Ye Jiao Teng* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9477 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.4526 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61750	61750	0.00	20.69
62051	62051	0.00	20.69
62052	62052	0.00	20.44
62131	62131	0.00	21.65
62132	62132	0.00	21.95

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Yi Mu Cao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60105-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Yi Mu Cao; Leonuri heterophylli herba

Special notes

When selecting the *Yi Mu Cao* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Yi Mu Cao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yi Mu Cao	G134H1050521	61671	40	from supplier
PhytoComm	Yi Mu Cao	G134H1050621	61983	40	from supplier
PhytoComm	Yi Mu Cao	G134H1050621	61984	40	from supplier

Validation samples

A total of 23 740 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 *Yi Mu Cao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 120 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 60 spectra from 3 reference samples of the substance/substance group *Yi Mu Cao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yi Mu Cao	G134H1050521	61671†	20
PhytoComm	Yi Mu Cao	G134H1050621	61983†	20
PhytoComm	Yi Mu Cao	G134H1050621	61984†	20

- 7389 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details

†These spectra were recorded from 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 the manufacturer and batch number mainly unchecked.

- 15 spectra from 9 *Apo-Ident* customers from 5 batches from the substance/substance group *Yi Mu Cao*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Yi Mu Cao	G134H1050521	1
PhytoComm	Yi Mu Cao	G134H1050521	3
PhytoComm	Yi Mu Cao	G134H1050023	3
Phytocomm	Yi Mu Cao	G134H1050023	1
Phytocomm	Yi Mu Cao	G134H1050024	3
PhytoComm	Yi Mu Cao	G134H1050024	1
Phytocomm	Yi Mu Cao	g134h1050024	1
PhytoComm	Yi Mu Cao	G134H1050321	2

- 2036 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Yi Mu Cao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yi Mu Cao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 120
Type B	0	60	0	7389
Type C	0	4	11	2036

The substance/substance group *Yi Mu Cao* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.8992 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.4523 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61671	61671	0.00	17.27
61983	61983	0.00	11.57
61984	61984	0.00	12.16

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Yi Yi Ren**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60174-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Yi Yi Ren; Coicis semen

Special notes

When selecting the *Yi Yi Ren* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Yi Yi Ren*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yi Yi Ren	`G078H1701421`	`61095`	40	from supplier
PhytoComm	Yi Yi Ren	`G078H1701522`	`61791`	40	from supplier
PhytoComm	Yi Yi Ren	`G078H1701522`	`61817`	40	from supplier
PhytoComm	Yi Yi Ren	`G078H1701522`	`62067`	40	from supplier
PhytoComm	Yi Yi Ren	`G078H1701522`	`62068`	40	from supplier
PhytoComm	Yi Yi Ren	`G078H1701622`	`62097`	40	from supplier
PhytoComm	Yi Yi Ren	`G078H1701622`	`62098`	40	from supplier

Validation samples

A total of 23 740 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 *Yi Yi Ren*. These samples are listed above in the section *calibration samples*. The reference samples originate from 3 different batches.

- 13 960 spectra from a total of 175 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 140 spectra from 7 reference samples of the substance/substance group *Yi Yi Ren*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yi Yi Ren	G078H1701421	61095†	20
PhytoComm	Yi Yi Ren	G078H1701522	61791†	20
PhytoComm	Yi Yi Ren	G078H1701522	61817†	20
PhytoComm	Yi Yi Ren	G078H1701522	62067†	20
PhytoComm	Yi Yi Ren	G078H1701522	62068†	20
PhytoComm	Yi Yi Ren	G078H1701622	62097†	20
PhytoComm	Yi Yi Ren	G078H1701622	62098†	20

- 7309 spectra from a total of 178 batches from further 143 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 25 spectra from 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Yi Yi Ren*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Yi Yi Ren	G078H1701522	3
Phytocomm	Yi Yi Ren	G078H1701222	3
PhytoComm	Yi Yi Ren	G078H1701323	7
Phytocomm	Yi Yi Ren	G078H1701323	1
Phytocomm	Yi Yi Ren	g078h1701323	1
Phytocomm	Yi Yi Ren	H1701021	8
PhytoComm	Yi Yi Ren	H1701021	1
PhytoComm	Yi Yi Ren	H1701923	1

- 2026 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Yi Yi Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yi Yi Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	13 960
Type B	0	140	0	7309
Type C	0	11	14	2026

The substance/substance group *Yi Yi Ren* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9477 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.8989 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.4520 %)	44.0000 % (> 32.0000 %)

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
61095	61095	0.00	42.92
61791	61791	0.00	41.11
61817	61817	0.00	40.31
62067	62067	0.00	36.47
62068	62068	0.00	37.15
62097	62097	0.00	40.05
62098	62098	0.00	39.57

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Yi Zhi Ren**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60172-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Yi Zhi Ren; Alpiniae fructus; Alpiniae oxyphyllae fructus

Special notes

When selecting the *Yi Zhi Ren* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Yi Zhi Ren*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yi Zhi Ren	G015H1051522	62185	40	from supplier
PhytoComm	Yi Zhi Ren	G015H1051522	62186	40	from supplier

Validation samples

A total of 23 740 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 *Yi Zhi Ren*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Yi Zhi Ren*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yi Zhi Ren	G015H1051522	62185†	20
PhytoComm	Yi Zhi Ren	G015H1051522	62186†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Yi Zhi Ren*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Yi Zhi Ren	G015H1051022	2
Herbasinica	Yi Zhi Ren	G015H1051321	1
Phytocomm	Yi Zhi Ren	G015H1051321	1
Phytocomm	Yi Zhi Ren	G015H1051521	1
PhytoComm	Yi Zhi Ren	G015H1051321	1

- 2045 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Yi Zhi Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yi Zhi Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	1	40	0	7408
Type C	1	3	3	2044

The substance/substance group *Yi Zhi Ren* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	99.9913 % (> 99.9410 %)	100.0000 % (> 85.0000 %)
Type C	99.9661 % (> 99.6926 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62185	62185	0.00	7.65
62186	62186	0.00	7.77

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Yin Chen Hao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60163-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Yin Chen Hao; Artemisiae scopariae herba

Special notes

When selecting the *Yin Chen Hao* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Yin Chen Hao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yin Chen Hao	G034H1030621	61832	40	from supplier

Validation samples

A total of 23 740 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 *Yin Chen Hao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Yin Chen Hao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yin Chen Hao	G034H1030621	61832†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Yin Chen Hao*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Fagron	Yin Chen Hao	G034H1030421	2
PhytoComm	Yin Chen Hao	G034H1030022	1
Phytocomm	Yin Chen Hao	G034H1030022	1
Phytocomm	Yin Chen Hao	G034H1030121	3
PhytoComm	Yin Chen Hao	G034H1030121	1
PhytoComm	Yin Chen Hao	H1030021	1
Phytocomm	Yin Chen Hao	H1030021	1

- 2041 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Yin Chen Hao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yin Chen Hao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	0	0	10	2041

The substance/substance group *Yin Chen Hao* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61832	61832	0.00	10.74

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Yin Yang Huo**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60228-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Yin Yang Huo; Epimedii herba

Special notes

When selecting the *Yin Yang Huo* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Yin Yang Huo*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yin Yang Huo	G098H1114621	61774	40	from supplier
PhytoComm	Yin Yang Huo	G098H1114621	61827	40	from supplier
PhytoComm	Yin Yang Huo	G098H1114622	62221	40	from supplier
PhytoComm	Yin Yang Huo	G098H1114622	62222	40	from supplier

Validation samples

A total of 23 740 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 *Yin Yang Huo*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Yin Yang Huo*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yin Yang Huo	G098H1114621	61774†	20
PhytoComm	Yin Yang Huo	G098H1114621	61827†	20
PhytoComm	Yin Yang Huo	G098H1114622	62221†	20
PhytoComm	Yin Yang Huo	G098H1114622	62222†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 10 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Yin Yang Huo*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phythocom	Yin Yang Huo	G098H1114222	1
PhytoComm	Yin Yang Huo	G098H1114121	2
Phytocomm	Yin Yang Huo	G098H1114422	2
phytocomm	Yin Yang Huo	FA1114702	1
Phytocomm	Yin Yang Huo	G098H1114121	1
PhytoComm	Yin Yang Huo	G098H1114222	1
Phytocomm	Yin Yang Huo	G098H1114222	1
PhytoComm	Yin Yang Huo	H1114923	1

- 2041 spectra from 17 *Apo-Ident* customers from a total of 969 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Yin Yang Huo* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yin Yang Huo* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 080
Type B	0	80	0	7369
Type C	0	1	9	2041

The substance/substance group *Yin Yang Huo* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4525 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61774	61774	0.00	10.57
61827	61827	0.00	10.73
62221	62221	0.00	12.21
62222	62222	0.00	11.80

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Yu Xing Cao**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60606-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Yu Xing Cao; Houttuyniae herba

Special notes

When selecting the *Yu Xing Cao* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Yu Xing Cao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yu Xing Cao	G124H1149423	61662	40	from supplier

Validation samples

A total of 23 740 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 *Yu Xing Cao*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Yu Xing Cao*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yu Xing Cao	G124H1149423	61662†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 6 *Apo-Ident* customers from 7 batches from the substance/substance group *Yu Xing Cao*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Yu Xing Cao	g124h1149222	1
Phytocomm	Yu Xing Cao	G124H1149222	1
Phytocomm	Yu Xing Cao	G124H1149423	2
Phytocomm	Yu Xing Cao	612yxc	1
Phytocomm	Yu Xing Cao	G124H1149122	5
Phytocomm	Yu Xing Cao	g124h1149122	1
PhytoComm	Yu Xing Cao	H1149821	1

- 2039 spectra from 17 *Apo-Ident* customers from a total of 967 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Yu Xing Cao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yu Xing Cao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	1	0	12	2038

The substance/substance group *Yu Xing Cao* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	99.9534 % (> 99.6796 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61662	61662	0.00	11.51

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Yuan Zhi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60100-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Yuan Zhi; Polygalae radix

Special notes

When selecting the *Yuan Zhi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Yuan Zhi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yuan Zhi	G194H1406622	62251	40	from supplier
PhytoComm	Yuan Zhi	G194H1406622	62252	40	from supplier

Validation samples

A total of 23 740 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 *Yuan Zhi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Yuan Zhi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yuan Zhi	G194H1406622	62251†	20
PhytoComm	Yuan Zhi	G194H1406622	62252†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 9 spectra from 8 *Apo-Ident* customers from 6 batches from the substance/substance group *Yuan Zhi*.

- These include spectra of independent samples from 6 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phythocom	Yuan Zhi	g194h1406222	1
Phytocomm	Yuan Zhi	G194H1406522	2
Phytocomm	Yuan Zhi	421401802	1
Phytocomm	Yuan Zhi	g194h140622	1
Phytocomm	Yuan Zhi	G194H1406222	2
PhytoComm	Yuan Zhi	G194H1406222	1
PhytoComm	Yuan Zhi	H1406924	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Yuan Zhi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yuan Zhi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	2	7	2041

The substance/substance group *Yuan Zhi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9534 % (> 99.6797 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62251	62251	0.00	9.94
62252	62252	0.00	9.91

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Ze Xie**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60165-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ze Xie; Alismatis rhizoma

Special notes

When selecting the *Ze Xie* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ze Xie*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ze Xie	`G011H1605521`	`61736`	40	from supplier

Validation samples

A total of 23 740 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 *Ze Xie*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Ze Xie*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ze Xie	G011H1605521	61736†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 6 batches from the substance/substance group *Ze Xie*.

- These include spectra of independent samples from 5 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Ze Xie	(G011)H1605122	1
Phytocomm	Ze Xie	G011H1605422	1
Phytocomm	Ze Xie	G011H1605521	5
PhytoComm	Ze Xie	G011H1605122	1
Phytocomm	Ze Xie	g011h1605122	1
PhytoComm	Ze Xie	H1605022	3
Phytocomm	Ze Xie	H1605022	1

- 2038 spectra from 17 *Apo-Ident* customers from a total of 968 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ze Xie* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ze Xie* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	2	5	8	2036

The substance/substance group *Ze Xie* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	99.8653 % (> 99.5914 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61736	61736	0.00	8.22

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Zhe Bei Mu**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	50388-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zhe Bei Mu; Fritillariae thunbergii bulbus

Special notes

When selecting the *Zhe Bei Mu* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zhe Bei Mu*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Zhe Bei Mu	G108H0712721	62217	40	from supplier
PhytoComm	Zhe Bei Mu	G108H0712721	62218	40	from supplier

Validation samples

A total of 23 740 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 *Zhe Bei Mu*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Zhe Bei Mu*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhe Bei Mu	G108H0712721	62217†	20
PhytoComm	Zhe Bei Mu	G108H0712721	62218†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Zhe Bei Mu*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Zhe Bei Mu	G108H0712121	7
PhytoComm	Zhe Bei Mu	G108H0712121	2
PhytoComm	Zhe Bei Mu	G108H0712321	2
Phytocomm	Zhe Bei Mu	G108H0712422	1

- 2039 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zhe Bei Mu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zhe Bei Mu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	12	2039

The substance/substance group *Zhe Bei Mu* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4524 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62217	62217	0.00	30.55
62218	62218	0.00	30.78

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Zhi Mu**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60196-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zhi Mu; Anemarrhenae radix; Anemarrhenae rhizoma

Special notes

When selecting the *Zhi Mu* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zhi Mu*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Zhi Mu	G019HS153QL1	62193	40	from supplier
PhytoComm	Zhi Mu	G019HS153QL1	62194	40	from supplier

Validation samples

A total of 23 740 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 *Zhi Mu*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Zhi Mu*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhi Mu	G019HS153QL1	62193†	20
PhytoComm	Zhi Mu	G019HS153QL1	62194†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 7 spectra from 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Zhi Mu*.

- These include spectra of independent samples from 3 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Zhi Mu	G019H0824221	1
PhytoComm	Zhi Mu	G019H0824321	2
PhytoComm	Zhi Mu	H0824922	2
Phytocomm	Zhi Mu	H0824922	2

- 2044 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zhi Mu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zhi Mu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	0	0	7	2044

The substance/substance group *Zhi Mu* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4529 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62193	62193	0.00	20.53
62194	62194	0.00	20.50

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Zhi Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60367-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zhi Zi; Gardeniae fructus

Special notes

When selecting the *Zhi Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zhi Zi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Zhi Zi	G110H1137521	61686	40	from supplier

Validation samples

A total of 23 740 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 *Zhi Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *Zhi Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhi Zi	G110H1137521	61686†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 11 spectra from 11 *Apo-Ident* customers from 3 batches from the substance/substance group *Zhi Zi*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phythocom	Zhi Zi	g110h1137121	1
Phytocomm	Zhi Zi	G110H1137521	3
PhytoComm	Zhi Zi	G110H1137521	1
phytocomm	Zhi Zi	G110H1137121	1
Phytocomm	Zhi Zi	G110H1137121	1
PhytoComm	Zhi Zi	G110H1137121	3
Phytocomm	Zhi Zi	g110h1137121	1

- 2040 spectra from 17 *Apo-Ident* customers from a total of 971 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zhi Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zhi Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	1	4	7	2039

The substance/substance group *Zhi Zi* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	99.9467 % (> 99.6729 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61686	61686	0.00	14.07

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Zhu Ru**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60241-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zhu Ru; Bambusae in taeniae caulis

Special notes

When selecting the *Zhu Ru* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zhu Ru*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Zhu Ru	`G047H0625621`	62025	40	from supplier
PhytoComm	Zhu Ru	`G047H0625621`	62026	40	from supplier
PhytoComm	Zhu Ru	`G047HS109QM2`	62207	40	from supplier
PhytoComm	Zhu Ru	`G047HS109QM2`	62208	40	from supplier

Validation samples

A total of 23 740 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 *Zhu Ru*. These samples are listed above in the section *calibration samples*. The reference samples originate from 2 different batches.

- 14 080 spectra from a total of 176 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *Zhu Ru*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhu Ru	G047H0625621	62025†	20
PhytoComm	Zhu Ru	G047H0625621	62026†	20
PhytoComm	Zhu Ru	G047HS109QM2	62207†	20
PhytoComm	Zhu Ru	G047HS109QM2	62208†	20

- 7369 spectra from a total of 179 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 15 spectra from 8 *Apo-Ident* customers from 7 batches from the substance/substance group *Zhu Ru*.

- These include spectra of independent samples from 7 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	Zhu Ru	G047H0625422	3
Phytocomm	Zhu Ru		1
PhytoComm	Zhu Ru	G047H0625121	1
Phytocomm	Zhu Ru	G047H0625122	1
PhytoComm	Zhu Ru	G047H0625122	1
PhytoComm	Zhu Ru	G047H0625321	2
Phytocomm	Zhu Ru	G047H0625321	3
Phytocomm	Zhu Ru	g047h0625321	1
phytocomm	Zhu Ru	g047h0625321	1
Phytocomm	Zhu Ru	G047h625321	1

- 2036 spectra from 17 *Apo-Ident* customers from a total of 967 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zhu Ru* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zhu Ru* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	1	14080
Type B	0	80	0	7369
Type C	0	2	13	2036

The substance/substance group *Zhu Ru* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	99.3750 % (> 97.5000 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4523 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62025	62025	0.00	11.37
62026	62026	0.00	12.26
62207	62207	0.00	5.90
62208	62208	0.00	5.90

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Zi Hua Di Ding**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`50376-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zi Hua Di Ding; Violae herba

Special notes

When selecting the *Zi Hua Di Ding* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zi Hua Di Ding*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Zi Hua Di Ding	`G249H1216621`	`61901`	40	from supplier
PhytoComm	Zi Hua Di Ding	`G249H1216621`	`61902`	40	from supplier

Validation samples

A total of 23 740 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 *Zi Hua Di Ding*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Zi Hua Di Ding*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zi Hua Di Ding	G249H1216621	61901†	20
PhytoComm	Zi Hua Di Ding	G249H1216621	61902†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 2 batches from the substance/substance group *Zi Hua Di Ding*.

- These include spectra of independent samples from 2 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Zi Hua Di Ding	G249H1216121	2
PhytoComm	Zi Hua Di Ding	G249H1216321	2

- 2047 spectra from 17 *Apo-Ident* customers from a total of 972 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zi Hua Di Ding* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zi Hua Di Ding* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	4	0	4	2043

The substance/substance group *Zi Hua Di Ding* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.8934 % (> 99.6203 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61901	61901	0.00	14.08
61902	61902	0.00	13.67

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Zi Su Zi**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60133-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zi Su Zi; Perillae fructus

Special notes

When selecting the *Zi Su Zi* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zi Su Zi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Zi Su Zi	G183H1213621	61933	40	from supplier
PhytoComm	Zi Su Zi	G183H1213621	61934	40	from supplier

Validation samples

A total of 23 740 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 *Zi Su Zi*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Zi Su Zi*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zi Su Zi	G183H1213621	61933†	20
PhytoComm	Zi Su Zi	G183H1213621	61934†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from 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 *Zi Su Zi*.

- These include spectra of independent samples from 1 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	Zi Su Zi	H1213921	1

- 2050 spectra from 17 *Apo-Ident* customers from a total of 973 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zi Su Zi* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zi Su Zi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14160
Type B	0	40	0	7409
Type C	0	0	1	2050

The substance/substance group *Zi Su Zi* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.4601 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61933	61933	0.00	16.66
61934	61934	0.00	16.68

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**Zi Wan**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`60155-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zi Wan; Asteris tatarici radix

Special notes

When selecting the *Zi Wan* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zi Wan*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Zi Wan	`G038H1215621`	`62045`	40	from supplier
PhytoComm	Zi Wan	`G038H1215621`	`62046`	40	from supplier

Validation samples

A total of 23 740 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 *Zi Wan*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *Zi Wan*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zi Wan	G038H1215621	62045†	20
PhytoComm	Zi Wan	G038H1215621	62046†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 8 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Zi Wan*.

- These include spectra of independent samples from 4 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
phytocomm	Zi Wan	g038h1215022	1
Phytocomm	Zi Wan	G038H1215321	2
PhytoComm	Zi Wan	G038H1215022	2
Phytocomm	Zi Wan	G038H1215022	1
Phytocomm	Zi Wan	H1215021	2

- 2043 spectra from 17 *Apo-Ident* customers from a total of 970 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zi Wan* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zi Wan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	1	2	6	2042

The substance/substance group *Zi Wan* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.9822 % (> 99.7086 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62045	62045	0.00	15.51
62046	62046	0.00	16.04

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**(Ku) Xing Ren**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	`50290-2018-10-23`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

(Ku) Xing Ren; Armeniacae amarum semen

Special notes

When selecting the *(Ku) Xing Ren* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *(Ku) Xing Ren*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	(Ku) Xing Ren	`G029H0708622`	`61838`	40	from supplier

Validation samples

A total of 23 740 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 *(Ku) Xing Ren*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 200 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 20 spectra from 1 reference samples of the substance/substance group *(Ku) Xing Ren*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	(Ku) Xing Ren	G029H0708622	61838†	20

- 7429 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 20 spectra from 9 *Apo-Ident* customers from 8 batches from the substance/substance group *(Ku) Xing Ren*.

- These include spectra of independent samples from 8 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
PhytoComm	(Ku) Xing Ren	G029H0708125	1
PhytoComm	(Ku) Xing Ren	G029H0708322	3
Phytocomm	(Ku) Xing Ren	161213xr	1
PhytoComm	(Ku) Xing Ren	G029H0708024	1
Phytocomm	(Ku) Xing Ren	G029H0708024	2
PhytoComm	(Ku) Xing Ren	G029H0708122	1
Phytocomm	(Ku) Xing Ren	G029H0708122	4
Phytocomm	(Ku) Xing Ren	g029h0708122	1
Phytocomm	(Ku) Xing Ren	G029H0708125	3
phytocomm	(Ku) Xing Ren	g029h0708322	2
PhytoComm	(Ku) Xing Ren	G029H708125	1

- 2031 spectra from 17 *Apo-Ident* customers from a total of 966 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *(Ku) Xing Ren* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *(Ku) Xing Ren* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 200
Type B	0	20	0	7429
Type C	0	0	20	2031

The substance/substance group *(Ku) Xing Ren* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9483 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9001 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.4521 %)	0.0000 % (≥ 0.0000 %)

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
61838	61838	0.00	68.21

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**(Sheng) Di Huang**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60005-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

(Sheng) Di Huang; Rehmanniae radix; Rehmanniae viridae radix

Special notes

When selecting the *(Sheng) Di Huang* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *(Sheng) Di Huang*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	(Sheng) Di Huang	G211H0532621	61797	40	from supplier
PhytoComm	(Sheng) Di Huang	G211H0532621	61804	40	from supplier
PhytoComm	(Sheng) Di Huang	G211H0532621	61881	40	from supplier
PhytoComm	(Sheng) Di Huang	G211H0532621	61882	40	from supplier

Validation samples

A total of 23 740 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 *(Sheng) Di Huang*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 080 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 80 spectra from 4 reference samples of the substance/substance group *(Sheng) Di Huang*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	(Sheng) Di Huang	G211H0532621	61797†	20
PhytoComm	(Sheng) Di Huang	G211H0532621	61804†	20
PhytoComm	(Sheng) Di Huang	G211H0532621	61881†	20
PhytoComm	(Sheng) Di Huang	G211H0532621	61882†	20

- 7369 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in 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 from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

- 19 spectra from 8 *Apo-Ident* customers from 7 batches from the substance/substance group *(Sheng) Di Huang*.

- These include spectra of independent samples from 7 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	(Sheng) Di Huang	G211H0532521	4
	(Sheng) Di Huang	g211h0532323	1
PhytoComm	(Sheng) Di Huang	G211H0532121	2
PhytoComm	(Sheng) Di Huang	G211H0532323	1
phytocomm	(Sheng) Di Huang	G211H0532121	1
Phytocomm	(Sheng) Di Huang	G211H0532121	3
Phytocomm	(Sheng) Di Huang	g211h0532121	1
Phytocomm	(Sheng) Di Huang	g211h053221	1
Phytocomm	(Sheng) Di Huang	G211H0532221	4
PhytoComm	(Sheng) Di Huang	G211H0532221	1

- 2032 spectra from 17 *Apo-Ident* customers from a total of 967 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *(Sheng) Di Huang* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *(Sheng) Di Huang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14080
Type B	0	80	0	7369
Type C	0	6	13	2032

The substance/substance group *(Sheng) Di Huang* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9478 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.8990 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.4522 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61797	61797	0.00	12.41
61804	61804	0.00	11.24
61881	61881	0.00	11.84
61882	61882	0.00	11.46

VALIDATION REPORT

IdentModul 1.3-2018-07

Validated substance/substance group	**(Shi) Chang Pu**
Substance class	TCM - Granulated herbal extracts (PhytoComm)
Report date	23/10/2018
Report number	60426-2018-10-23
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

(Shi) Chang Pu; Acori graminei rhizoma; Acori rhizoma

Special notes

When selecting the *(Shi) Chang Pu* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	*European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*
Anhang F	Zusatz zu den Modellen der zweiten Stufe

Validation method

Validation occurs after every change to the chemometric model (also "database ") and does so in two steps:

1. The chemometric model is calculated from the calibration spectra using a PCA algorithm. The calibration spectra originate from the calibration samples of all substances in this class.

2. The generated chemometric model is presented all appropriate spectra for evaluation. In three runs, the reference spectra (*Type A*) are presented spectra from independent (*Type B*) samples and spectra from the (*Type C*) field successively.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *(Shi) Chang Pu*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	(Shi) Chang Pu	G006H0544622	62107	40	from supplier
PhytoComm	(Shi) Chang Pu	G006H0544622	62108	40	from supplier

Validation samples

A total of 23 740 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 *(Shi) Chang Pu*. These samples are listed above in the section *calibration samples*. The reference samples originate from 1 different batches.

- 14 160 spectra from a total of 177 batches from further 140 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database.

Samples from batches, from which no spectra have been used for the generation of the database are considered as independent samples. The number of batches from which independent samples have delivered *Type B* spectra for the validation is given below and thus represents the number of independent *Type B* samples. Samples from which a number of the spectra has been used for the generation of the database and other spectra have been incorporated into the validation, are marked with a †. The following applies to the remaining unmarked samples: There was at least one other sample from the same batch (other sales containers, other sample ID), of which reference spectra (*Type A*) were used for the generation of the database.

- 40 spectra from 2 reference samples of the substance/substance group *(Shi) Chang Pu*.

- These include spectra of independent samples from 0 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	(Shi) Chang Pu	G006H0544622	62107†	20
PhytoComm	(Shi) Chang Pu	G006H0544622	62108†	20

- 7409 spectra from a total of 180 batches from further 143 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra from the field, which were not recorded under of the control of *Hiperscan GmbH* and have not been used for the generation of the database. *Hiperscan GmbH* accepts the details provided by the customer regarding the manufacturer and batch number mainly unchecked.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 9 spectra from 5 *Apo-Ident* customers from 7 batches from the substance/substance group *(Shi) Chang Pu*.

- These include spectra of independent samples from 7 batches, of which no spectra have been used for the generation of the database.

Supplier	Substance	Batch	Spectra
Phytocomm	(Shi) Chang Pu	G006HS270ON1	1
PhytoComm	(Shi) Chang Pu	G006H0544023	1
Phytocomm	(Shi) Chang Pu	G006H0544122	3
Phytocomm	(Shi) Chang Pu	g006h0544023	1
Phytocomm	(Shi) Chang Pu	G006H0544321	1
Herbasinica	(Shi) Chang Pu	g006h0544321	1
Phytocomm	(Shi) Chang Pu	G006H0544322	1

- 2042 spectra from 17 *Apo-Ident* customers from a total of 967 batches from a further 267 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *(Shi) Chang Pu* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *(Shi) Chang Pu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	14 160
Type B	0	40	0	7409
Type C	14	0	9	2028

The substance/substance group *(Shi) Chang Pu* can be distinguished from other substances with some limitations. (*False-positive* classifications were obtained.) In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9479 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.8994 %)	100.0000 % (> 85.0000 %)
Type C	99.5334 % (> 99.2597 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62107	62107	0.00	10.41
62108	62108	0.00	11.69

Appendix A: Additional calibration samples (*Type A*)

Not required.

Appendix B: Additional validation samples (*Type B*)

It is necessary that spectra also enter the validation which cannot be identified with this model. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded by *HiperScan GmbH*. They are allocated to the *Type B*. They also include the calibration spectra for other models.

The samples originate from 6 batches. From these 240 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
PhytoComm	Mang Xiao	G160H0627623	45	from supplier
PhytoComm	Mang Xiao	G160H0627623	45	from supplier
PhytoComm	Mu Li (Sheng)	G178HS128PN1	30	from supplier
PhytoComm	Mu Li (Sheng)	G178HS128PN1	30	from supplier
PhytoComm	Shi Gao	G120H0541721	45	from supplier
PhytoComm	Shi Gao	G120H0541721	45	from supplier

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 386 batches. From these, 736 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
Bios	Lu Hui	424263	3
Caelo	Bai Guo	g114h0509022	1
EuRho	Dang Shen	g077h2001222	2
Herba Natura	Qu Mai	8950	1
Herbasin	Hua Shi	G238H332121	1
Herbasin	Huang Qin	g225h120442	1
Herbasin	Sha Shen (Bei)	G117H0754121	8
Mediherb	Zhu Ling		1
phythocom	Hong Hua	g057h0901121	2
phythocom	Lu Jiao Shuang	G062H1419321	1
phythocom	Ren Shen	115h562121	1
phythocom	Ren Shen	g115h0562121	1
phythocom	She Chuang Zi	G076H1154122	3
phythocom	Shi Gao	G120H0541223	7
phythocom	Tian Men Dong	g037h0415021	1
phytocomm	Bai Bu	G235H0608021	1
phytocomm	Bai Guo	G114H0509022	1
phytocomm	Bai Qian	BP010536	1
phytocomm	Ce Bai Ye	g050h0975321	2
phytocomm	Chan Tui	g067h1817322	1
phytocomm	Chi Shao (Yao)	G180H0705121	3
phytocomm	Chuan Mu Tong	G009H0310121	5
phytocomm	Chuang Mu Xiang	G219H0309021	2
phytocomm	Di Long	g148h603321	1
phytocomm	E Bu Shi Cao	G061H1801022	3
phytocomm	E Jiao	G036H0861022	2
phytocomm	Gu Ya	G177H1513021	2
phytocomm	Hai Piao Xiao	G305BP051026	1
phytocomm	Hu Zhang	G197H0851021	2
phytocomm	Huo Xiang	H2005021	5
phytocomm	Jue Ming Zi	G059H1097121	2
phytocomm	Lu Jiao Jiao	g323h1158121	1
phytocomm	Lu Rong	G296BP031136	1
phytocomm	Mang Xiao	G160H0627121	1
phytocomm	Mi Meng Hua	G054BP021404	2
phytocomm	Pu Huang	H1316021	2
phytocomm	Shi Gao	g120h541024	1
phytocomm	Suo Yang	G260H1439022	1
phytocomm	Wu Gong	G311H1411021	3
phytocomm	Wu Mei	H1026021	4
phytocomm	Xi Xian Cao	G229H1431121	7
phytocomm	Xian He Cao	g008h0547321	1
phytocomm	Ye Ju Hua	G514H1187021	3
phytocomm	Zhi Shi	g044h0922321	1
phytocomm	Zhu Ling	G199H1509022	3
Phytocomm	(Bai) Dou Kou	GO16H0508521	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phytocomm	(Bai) Dou Kou	G016H0508521	1
Phytocomm	(Bai) Dou Kou	G016H0508021	1
Phytocomm	(Bai) Jiang Can	g269h0513222	1
Phytocomm	(Bai) Jiang Can	G269H0513321	2
Phytocomm	(Bai) Jiang Can	g144h1708221	1
Phytocomm	(Bai) Jiang Can	G269H0513222	3
Phytocomm	(Fen) Bi Xie	G290BP021212	1
Phytocomm	(Fen) Bi Xie	G290H1251121	3
Phytocomm	(Fen) Bi Xie	G29H1251121	1
Phytocomm	(Huai) Niu Xi	G003H1905122	2
Phytocomm	(Huai) Niu Xi	G003H1905321	2
Phytocomm	(Huai) Niu Xi	G003H1905222	4
Phytocomm	(Huai) Niu Xi	G003H1905422	2
Phytocomm	(Huai) Niu Xi	g003h1905222	1
Phytocomm	Bai Bu	H0608921	1
Phytocomm	Bai Bu	G235H0608321	1
Phytocomm	Bai Bu	G235H0608121	2
Phytocomm	Bai Guo	G114H0509521	1
Phytocomm	Bai Guo	G114H0509321	2
Phytocomm	Bai Jiang Cao	G181H1180321	1
Phytocomm	Bai Jiang Cao	G181H1180422	1
Phytocomm	Bai Jie Zi	H0518921	1
Phytocomm	Bai Mao Gen	G125H0512221	2
Phytocomm	Bai Qian	G087H0505922	3
Phytocomm	Bai Tou Weng	G207H0511521	4
Phytocomm	Bai Tou Weng	G207H0511221	3
Phytocomm	Bai Zhi	G020H0503223	1
Phytocomm	Bai Zhi	G020H0503421	1
Phytocomm	Bai Zhi	G020H0503122	2
Phytocomm	Bing Lang	G027H1825221	2
Phytocomm	Bo He	g158h1712022	1
Phytocomm	Bo He	G158H1712121	2
Phytocomm	Bo He	G158H1712022	5
Phytocomm	Ce Bai Ye	G050H0975321	1
Phytocomm	Ce Bai Ye	G050HS245	1
Phytocomm	Chan Tui	G067H1817323	2
Phytocomm	Chan Tui	G067H1817121	2
Phytocomm	Chi Shao (Yao)	G189H0705321	1
Phytocomm	Chi Shao (Yao)	G180H0705422	1
Phytocomm	Chi Shao (Yao)	G180H705121	1
Phytocomm	Chi Shao (Yao)	G180H0705321	2
Phytocomm	Chi Shao (Yao)	g180h0705122	1
Phytocomm	Chong Wei Zi	G317BP021046	1
Phytocomm	Chong Wei Zi	g317bp021046	1
Phytocomm	Chuan Bei Mu	g107f11021	1
Phytocomm	Chuan Bei Mu	g107f110721	2
Phytocomm	Chuan Bei Mu	G107BP020722A	2
Phytocomm	Chuan Mu Tong	g009h0310321	1
Phytocomm	Chuan Mu Tong	G009H0310321	1
Phytocomm	Chuang Mu Xiang	G219H0309521	2
Phytocomm	Chuang Mu Xiang	G219H0309322	1
Phytocomm	Chuang Mu Xiang	g219h0309321	1
Phytocomm	Chuang Mu Xiang	g219h0309322	1
Phytocomm	Da Fu Pi	G293H0321021	1
Phytocomm	Da Fu Pi	G293H0321122	2
Phytocomm	Da Fu Pi	G293H0321221	1
Phytocomm	Dang Shen	G077H2001222	2
Phytocomm	Dang Shen	G077H2001521	4
Phytocomm	Deng Xin Cao	f100707	1
Phytocomm	Deng Xin Cao	G306F100617	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phytocomm	Di Long	G148H0603421	2
Phytocomm	Di Long	G148H0603022	3
Phytocomm	Di Long	G148H0603321	2
Phytocomm	Di Yu	G2150604121	1
Phytocomm	Di Yu	G215H0604322	2
Phytocomm	Ding Xiang	G058H0210021	1
Phytocomm	Ding Xiang	H0210921	1
Phytocomm	Du Huo	G021H1610421	2
Phytocomm	Du Huo	g021h610221	1
Phytocomm	Du Huo	421605602	2
Phytocomm	Du Zhong	G101H0736522	5
Phytocomm	Du Zhong	H0736923	1
Phytocomm	Du Zhong	g101h0736021	1
Phytocomm	Du Zhong	G101H0736321	2
Phytocomm	Du Zhong	g101h076521	1
Phytocomm	E Bu Shi Cao	G061H1801122	2
Phytocomm	E Jiao	G036H0861421	2
Phytocomm	E Jiao	g036h0861121	1
Phytocomm	E Jiao	g036h0861221	1
Phytocomm	Fu Shen	g201h1021321	1
Phytocomm	Fu Shen	G201H1021321	3
Phytocomm	Fu Shen	G201H1021422	2
Phytocomm	Gou Teng	g247h1210122	1
Phytocomm	Gou Teng	612gt	1
Phytocomm	Gou Teng	H1210021	1
Phytocomm	Gou Teng	G247H1210422	2
Phytocomm	Hai Tong Pi	G100H1076221	2
Phytocomm	Han Lian Cao	G095H0770521	4
Phytocomm	Han Lian Cao	g095h0770321	1
Phytocomm	Han Lian Cao	G095H0770321	3
Phytocomm	He Shou Wu	g198h0718222	1
Phytocomm	He Shou Wu	H0718021	2
Phytocomm	He Shou Wu	G198H0718222	2
Phytocomm	He Shou Wu	G198H0718421	3
Phytocomm	He Zi	G291H1239021	2
Phytocomm	He Zi	G291H1239221	3
Phytocomm	Hong Hua	G057H0901221	2
Phytocomm	Hong Hua	G057H0901322	1
Phytocomm	Hong Hua	41024032/2	1
Phytocomm	Hu Zhang	G197H0851321	2
Phytocomm	Hu Zhang	g197h0851321	1
Phytocomm	Hua Shi	G238H1332121	3
Phytocomm	Hua Shi	g238h1332121	1
Phytocomm	Huang Qin	G225H1204221	4
Phytocomm	Huang Qin	G225H1204522	3
Phytocomm	Huang Qin	161213hq	1
Phytocomm	Huang Qin	G225H1204121	5
Phytocomm	Huang Qin	g225h1204121	1
Phytocomm	Huo Ma Ren	G141HS061	1
Phytocomm	Ji Li	H0858021	2
Phytocomm	Ji Li	G240H1410421	1
Phytocomm	Ji Nei Jin	g259h2102321	1
Phytocomm	Ji Xue Teng	G159H2101423	3
Phytocomm	Ji Xue Teng	G159H2101122	5
Phytocomm	Ji Xue Teng	g159h2101122	1
Phytocomm	Ji Xue Teng	H2101923	1
Phytocomm	Jie Cao	H2111921	1
Phytocomm	Jin Qian Cao	G1514H0847122	1
Phytocomm	Jin Qian Cao	g151h0847122	1
Phytocomm	Jin Ying Zi	G023H0317921	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phytocomm	Jin Ying Zi	G023H0846221	1
Phytocomm	Ju Hong	G310H1623121	2
Phytocomm	Jue Ming Zi	G059H1097221	3
Phytocomm	Jue Ming Zi	G059H1097023	1
Phytocomm	Ling Zhi	g109fb2405321	1
Phytocomm	Long Gu	g0251706122	1
Phytocomm	Lu Gen	G189H2014521	3
Phytocomm	Lu Gen	F100708	3
Phytocomm	Lu Jiao Jiao	G323H1158022	1
Phytocomm	Lu Jiao Shuang	FB1419901	2
Phytocomm	Lu Jiao Shuang	G062H1419421	1
Phytocomm	Ma Bian Cao	G248H1085221	1
Phytocomm	Mi Huan Jun	G510H0418422	1
Phytocomm	Mi Huan Jun	G510H0418221	1
Phytocomm	Mi Huan Jun	G510H110164	2
Phytocomm	Mu Li (Sheng)	G178H0740221	2
Phytocomm	Mu Zei	G265H0427421	1
Phytocomm	Mu Zei	G265H0427823	2
Phytocomm	Pang Da Hai	G529H0960023	2
Phytocomm	Qian Hu	H0926021	2
Phytocomm	Qian Hu	G185H0926322	4
Phytocomm	Qian Hu	G185H0926121	1
Phytocomm	Qian Shi	G102H0836422	1
Phytocomm	Qing Hao	G031H0810221	2
Phytocomm	Quan Xie	G222F110314	1
Phytocomm	Ren Shen	G1150562121	1
Phytocomm	Ren Shen	g115ho562121	1
Phytocomm	Sang Ji Shend	G146H1045522	4
Phytocomm	Sang Ji Shend	G146H1045222	2
Phytocomm	Sang Ji Shend	g146h1045222	1
Phytocomm	Sang Ji Shend	H1045021	2
Phytocomm	Sang Piao Xiao	G282H421029201	1
Phytocomm	Sang Shen	G163H1047121	2
Phytocomm	Sha Shen (Bei)	G117H0754322	3
Phytocomm	Shan Yao	G091H0330521	4
Phytocomm	Shi Gao	G120H051024	1
Phytocomm	Shi Gao	G120H0541024	11
Phytocomm	Shi Wei	H0543021	2
Phytocomm	Suo Yang	G260H1831121	2
Phytocomm	Tai Zi Shen	G204H0446521	1
Phytocomm	Tai Zi Shen	G204H0446221	2
Phytocomm	Tian Hua Fen	h0417022	2
Phytocomm	Tian Hua Fen	G242H0417522	2
Phytocomm	Tian Hua Fen	G242H0417423	1
Phytocomm	Tian Men Dong	G037H0415321	1
Phytocomm	Tian Men Dong	G037H0415221	1
Phytocomm	Tian Men Dong	g03h0415521	1
Phytocomm	Tian Men Dong	g037h0415221	1
Phytocomm	Tian Nan Xing	G028H0420922	2
Phytocomm	Ting Li Zi	H1340022	1
Phytocomm	Tong Cao	G531H1141021	1
Phytocomm	Tong Cao	G531H114021	2
Phytocomm	Wa Leng Zi	G508F110305	2
Phytocomm	Wu Gong	G311H411321	1
Phytocomm	Wu Gong	G311H1411321	1
Phytocomm	Wu Mei	G167H1026421	1
Phytocomm	Wu Mei	G167H1026221	1
Phytocomm	Wu Zhu Yu	G13H0766021	1
Phytocomm	Xi Xian Cao	G229H1431321	2
Phytocomm	Xian He Cao	G008H0547121	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phytocomm	Xian He Cao	G008H0547321	1
Phytocomm	Xian Mao	G304H0549521	2
Phytocomm	Xian Mao	G304H0549321	2
Phytocomm	Xiang Fu	G088H0930521	6
Phytocomm	Xiang Fu	go88h09	1
Phytocomm	Xiang Fu	g088h0930123	1
Phytocomm	Xiang Fu	G088H0930123	5
Phytocomm	Xue Jie	G322H0631921	1
Phytocomm	Yin Xing Ye	G518H1445021	1
Phytocomm	Yu Jin	422901803	1
Phytocomm	Yu Zhu	G195H0517421	2
Phytocomm	Ze Lan	g268h1606221	1
Phytocomm	Ze Lan	G268H1606421	1
Phytocomm	Zhen Zhu Mu	g155h0979221	1
Phytocomm	Zhi Gan Cao	G118H0881522	4
Phytocomm	Zhi Gan Cao	G118H0881221	2
Phytocomm	Zhi Gan Cao	g118h0881322	1
Phytocomm	Zhi Ke	G043H0921422	2
Phytocomm	Zhi Shi	g044h0922221	1
Phytocomm	Zhi Shi	G044H0922521	3
Phytocomm	Zhu Ling	G199H1509421	2
Phytocomm	Zi Su Ye	G182H1214321	3
PhytoComm	(Bai) Jiang Can	H0513021	3
PhytoComm	(Bai) Jiang Can	G269H0513121	2
PhytoComm	(Dai) Zhe Shi	410520701	1
PhytoComm	(Fen) Bi Xie	H1251921	1
PhytoComm	(Fen) Bi Xie	G0290H1251121	1
PhytoComm	(Huai) Niu Xi	H1905021	3
PhytoComm	(Huai) Niu Xi	G003H190522	1
PhytoComm	Bai Bu	G235H0608221	1
PhytoComm	Bai Jiang Cao	(G181)H1180022	1
PhytoComm	Bai Jiang Cao	G181H1180022	1
PhytoComm	Bai Zhi	G020H0503024	3
PhytoComm	Bie Jia	G507H2401121	3
PhytoComm	Bie Jia	G507H2401321	2
PhytoComm	Bing Lang	H1825021	4
PhytoComm	Cao Guo	E241050	1
PhytoComm	Ce Bai Ye	G050H0975021	2
PhytoComm	Chan Tui	G067H1817322	4
PhytoComm	Chan Tui	G06H1817121	1
PhytoComm	Chi Shao (Yao)	G180H0705122	4
PhytoComm	Chong Wei Zi	E341046	1
PhytoComm	Chuan Bei Mu	G107F110721	2
PhytoComm	Chuan Bei Mu	H0711921	1
PhytoComm	Chuan Mu Tong	H0310021	1
PhytoComm	Chuan Mu Tong	G009H0310521	1
PhytoComm	Chuan Xin Lian	G321FB0963321	1
PhytoComm	Chuan Xin Lian	H0963921	1
PhytoComm	Ci Shi	F100628	1
PhytoComm	Cong Bai	424348	2
PhytoComm	Da Fu Pi	H0321922	1
PhytoComm	Dang Shen	H2001021	3
PhytoComm	Dang Shen	g077H2001222	1
PhytoComm	Dang Shen	G077H2001022	2
PhytoComm	Deng Xin Cao	F100707	1
PhytoComm	Di Fu Zi	G131H0605021	1
PhytoComm	Di Fu Zi	G131H0605122	4
PhytoComm	Di Long	G148H603321	1
PhytoComm	Ding Xiang	G058h0210021	1
PhytoComm	Du Huo	H1610922	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
PhytoComm	Du Huo	G021H1610221	1
PhytoComm	Du Zhong	H0736021	3
PhytoComm	Du Zhong	G101H0736021	2
PhytoComm	E Bu Shi Cao	G061H180122	1
PhytoComm	E Jiao	G036H0861221	5
PhytoComm	E Jiao	G036H0861121	2
PhytoComm	Fu Shen	G201F110526	2
PhytoComm	Gao Ben	G137H1809221	1
PhytoComm	Gao Ben	H1809921	2
PhytoComm	Geng Mi	414161	1
PhytoComm	Geng Mi	G329H1320121	1
PhytoComm	Gou Teng	G247H1210122	4
PhytoComm	Gu Ya	H1513921	2
PhytoComm	Gui Ban	G530F110210	2
PhytoComm	Han Lian Cao	G095H0770121	4
PhytoComm	Han Lian Cao	G263H1423121	2
PhytoComm	He Shou Wu	(G198)H0718222	1
PhytoComm	He Ye	H1170922	1
PhytoComm	Hong Hua	G057H0901121	3
PhytoComm	Hu Zhang	G197H081021	1
PhytoComm	Hua Shi	G238H133121	1
PhytoComm	Huang Qin	G225H1204022	6
PhytoComm	Huang Qin	G225H1204322	6
PhytoComm	Huo Ma Ren	G141H0449121	2
PhytoComm	Ji Li	G240H1410221	1
PhytoComm	Ji Nei Jin	G259H2102023	3
PhytoComm	Ji Nei Jin	G259H2102321	2
PhytoComm	Ji Nei Jin	H2102021	1
PhytoComm	Jin Qian Cao	H0847921	2
PhytoComm	Jin Qian Cao	G151H0847922	3
PhytoComm	Jin Qian Cao	G151H0847122	3
PhytoComm	Jue Ming Zi	G059H1097221	2
PhytoComm	Ling Zhi	FA2405901	1
PhytoComm	Ling Zhi	G109F-B2405221	2
PhytoComm	Ling Zhi	G109FB2405321	1
PhytoComm	Long Gu	G025H1706122	1
PhytoComm	Lu Gen	G189H2014221	4
PhytoComm	Lu Jiao Jiao	G323H1158321	2
PhytoComm	Lu Jiao Jiao	G323H1158121	2
PhytoComm	Ma Chi Xian	G255F110310	3
PhytoComm	Mang Xiao	H0627021	1
PhytoComm	Mao Dong Qing	G319H0411121	1
PhytoComm	Mu Li (Sheng)	H0740922	2
PhytoComm	Mu Zei	H0427822	1
PhytoComm	Qian Shi	H0836921	1
PhytoComm	Qian Shi	G102H0836121	4
PhytoComm	Qing Hao	G031H0810021	2
PhytoComm	Ren Dong Teng	(G297)H075122	1
PhytoComm	Ren Dong Teng	G297H0751222	1
PhytoComm	Ren Dong Teng	H0751922	1
PhytoComm	Ren Shen	G115H0562121	1
PhytoComm	Rou Dou Kou	G16BP020616	1
PhytoComm	Sang Ji Shend	G146H1045322	2
PhytoComm	Sang Shen	G163H1047221	3
PhytoComm	Sang Shen	H1047921	1
PhytoComm	Shan Yao	H0330021	2
PhytoComm	Shan Yao	G091H0330122	1
PhytoComm	She Chuang Zi	G076H1154021	2
PhytoComm	Shi Jue Ming	H0546021	1
PhytoComm	Tian Hua Fen	H0417022	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
PhytoComm	Tian Hua Fen	G242H0417122	1
PhytoComm	Tian Men Dong	G037H0415021	2
PhytoComm	Tian Men Dong	G037H0415121	2
PhytoComm	Ting Li Zi	G135H1340121	1
PhytoComm	Wu Mei	G167H1026121	2
PhytoComm	Wu Zhu Yu	(G103)H0766321	1
PhytoComm	Wu Zhu Yu	G103H0766021	2
PhytoComm	Wu Zhu Yu	G103H0766321	3
PhytoComm	Wu Zhu Yu	G103H0766022	4
PhytoComm	Xian He Cao	H0547021	3
PhytoComm	Xian Mao	G304H0549021	3
PhytoComm	Xiang Fu	G088H0930321	2
PhytoComm	Xiang Fu	H0930021	2
PhytoComm	Ye Ju Hua	(G514)H1187021	1
PhytoComm	Yin Chai Hu	G368H1444221	1
PhytoComm	Yin Xing Ye	H1445921	1
PhytoComm	Yu Jin	G084H2201221	1
PhytoComm	Yu Jin	H2201021	2
PhytoComm	Yu Jin	G084H2201322	1
PhytoComm	Yu Li Ren	H0967922	1
PhytoComm	Yu Zhu	H0517022	3
PhytoComm	Yu Zhu	G195H0517321	1
PhytoComm	Yu Zhu	G195H0517121	1
PhytoComm	Ze Lan	G268H1606022	3
PhytoComm	Ze Lan	G268H1606221	2
PhytoComm	Ze Lan	G268H1606021	2
PhytoComm	Zhen Zhu Mu	H0979921	1
PhytoComm	Zhi Gan Cao	G118H0881122	3
PhytoComm	Zhi Gan Cao	G118H0881322	2
PhytoComm	Zhi Ke	G043H0921221	3
PhytoComm	Zhi Ke	H0921021	1
PhytoComm	Zhi Shi	G044H0922021	3
PhytoComm	Zhi Shi	G044H0922121	2
PhytoComm	Zhi Shi	G044H0922221	6
PhytoComm	Zhi Shi	G044H0922321	5
PhytoComm	Zhi Shi	H0922921	1
PhytoComm	Zhu Ling	G199H1509521	1
PhytoComm	Zi Su Ye	G182HS268OP1	1
PhytoComm	Zi Su Ye	G182H1214021	3
Sino Phyto	Long Gu	G025H1706122	4

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).

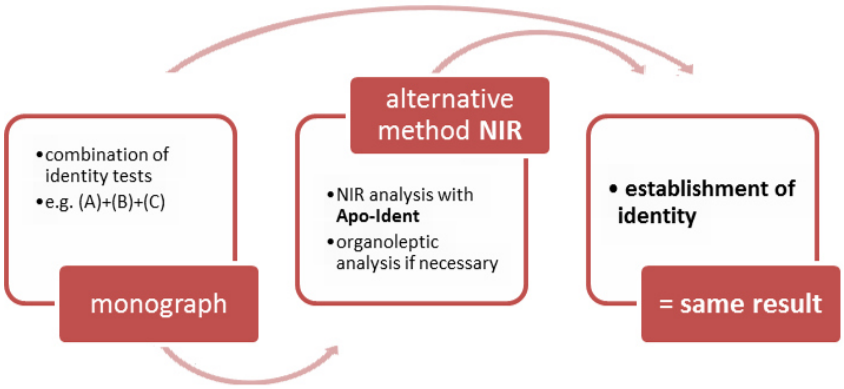

Figure 2: The combination of tests of the monograph is replaced by the alternative method NIR spectroscopy using *Apo-Ident*. This is permissible because both test procedures result in the establishment of the identity of the raw material.

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 2018-07*, a distinction is made between the following substances in the listed second-stage models:

Submodel 1

Bacitracin
Betamethasone, micronized
Betamethasone valerate
Budesonide, micronized
Capsaicin, natural
Dexamethasone
Erythromycin
Hydrocortisone butyrate
Norethisterone acetate
Prednicarbate, micronized
Prednisolone, 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 alcohol cream DAB/SR

References

[1] ABDA – Bundesvereinigung Deutscher Apothekerverbände: Verordnung über den Betrieb von Apotheken (Apothekenbetriebsordnung – ApBetrO), 2012

[2] Reimann, B. ; Regierungspräsidium Darmstadt: Hinweise zur ordnungsgemäßen Prüfung von Arzneimitteln und Ausgangsstoffen (§§ 6 und 11 *ApBetrO*), 2007

[3] *Europäisches Arzneibuch, Grundwerk 2014 einschließlich 1. bis 4. Nachtrag.* 8. Ausgabe. Deutscher Apotheker Verlag (978-3-7692-6508-8)

[4] HiperScan GmbH: Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident, 2013

[5] Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD): Resolution in Verbindung mit §§ 6 und 11 *ApBetrO* Verwendung eines Nah-Infrarot-Spektrometers (NIR) zur Identitätsprüfung, 16. 10. 2013, DAZ 48, November 2013

[6] Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD): Resolution 2014, Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD), Oktober 2014

[7] *DAC/NRF.* Govi-Verlag (978-3-7741-0044-2)

[8] Kessler, W.: *Multivariate Datenanalyse.* WILEY-VCH Verlag, 2007 (978-3-527-31262-7)

[9] Næs, T. ; Isaksson, T. ; Fearn, T. ; Davies, T.: *Multivariate Calibration and Classification.* NIR Publications, 2002 (978 0 9528666 2 6)

[10] Hanley, J. A. ; Lippman-Hand, A.: If nothing goes wrong, is everything all right? In: *Journal of the American Medical Association* 249 (1983), S. 1743–1745

[11] Jovanovic, B. D. ; Levy, P. S.: A Look at the Rule of Three. In: *The American Statistician* 51 (1997), S. 137–139

[12] Bronstein, I. N. ; Semendjajew, K. A. ; Musiol, G. ; Mühlig, H.: *Taschenbuch der Mathematik.* 5. überarbeitete und erweiterte Auflage. Verlag Harri Deutsch, 2000 (3-8171-2015-2)

[13] Mahalanobis, P.: On the generalized distance in statistics. In: *Proc. Nat. Inst. Sci. India (Calcutta)* 2 (1936), S. 49–55

[14] Yambor, B. ; Draper, W. ; Beveridge, R.: Analyzing PCA-based face recognition algorithms: Eigenvector selection and distance measures. In: *Second Workshop Empirical Evaluation in Computer Vision* (2000)

[15] HiperScan GmbH: Identifikationsmethodik Apo-Ident, 2012

[16] HiperScan GmbH: Datenvorbehandlung des Identifikationssystems Apo-Ident, 2012

[17] Cyran ; Rotta: Apothekenbetriebsordnung, Kommentar § 6 Rn. 10, 2010

Index