

Validation documentation
TCM - Granulated herbal extracts (PhytoComm)

HiperScan GmbH

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Introduction

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

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

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

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

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

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

Context of this document

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

- *NIR spectroscopy as a method for identity testing*: The *Ph. Eur.* [3] describes NIR spectroscopy in *Section 2.2.40* as an analytical method which is also suitable for the identification of raw materials. Therefore, validation of the method as such is not necessary.
- *Performance of the instrument*: The *Ph. Eur.* [3] furthermore describes the apparatus and the testing of its performance in *Section 2.2.40*. The document *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4] compares the implementation by *Apo-Ident* with this monograph in order to prove that *Apo-Ident* meets the specifications of the Pharmacopoeia. Each individual instrument delivered to a pharmacy is qualified in accordance with the tests described in “*Control of Instrument Performance*”. In this test, the unit consisting of analysis instrument hardware and the *QuickStep* spectroscopy software is assessed. The result is documented in a test protocol which is kept at the pharmacy.
- *Validation of the database* is documented separately for each substance class. The report at hand documents the substance class *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. Bezugsquellen-nachweis für Rezepturbestandteile* [Sources of supply for compounding] [7]).
- b) Testing the suitability according to *ApBetrO* [Pharmacies Rules and Regulations] §§ 6, 11, that is to say the availability of a valid manufacturer certificates via identity, purity and contents of the batch.
- c) Recording standard 40 spectra of the sample in different positions, as a standard on four instruments. Here, handling and presentation of the samples as later in the pharmacy.
- d) Visual checking for anomalies in the spectra. In case of indications of measurement errors, measurement must be repeated. If a signature is missing in the spectrum, the substance may be excluded from the start as not promising (the spectra are nonetheless entered in the database validation as independent *Type B* spectra).

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

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

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

2. Generating the chemometric models (calibration)

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

3. Set of validation spectra (validation samples)

The following is provided for validation:

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

All manufacturers’ batches from which spectra are used for the validation are listed by substance in this document: for substances included in the substance class *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 themselves and keeps the test certificates.

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

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

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

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

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

Significance of testing with *Apo-Ident*

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

Verbally, the statement of the analysis result can be expressed as follows. Here "*the spectra match*" means that the criteria *Mahalanobis distance*, *outlier analysis* and *correlation* are met as shown in *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]. "The spectra do not match", on the other hand, means that at least the criterion *Mahalanobis distance* is not met.

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

1. The spectrum of the sample measured matches spectra of the defined substance.

2. The spectrum of the sample measured does not match any spectrum of any other substance in this substance class. Therefore, all other substances can be clearly ruled-out.
3. As the spectra from other substance classes were used for validation, it is proven that no spectrum of one of these other substances matches the defined substance. (All substance classes with which a spectrum comparison is possible and makes sense are used for validation. This is documented for each substance class in the section [Summary](#).)
4. If the defined substance belongs to a [substance group](#) which in itself is not clearly separable with *Apo-Ident*, matching with the spectra of one or several substances in this group is confirmed. Which of these substances it actually is cannot be determined clearly. All other substances are excluded analogous to [2](#) and [3](#).

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

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

Conclusion

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

Explanation of terminology

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

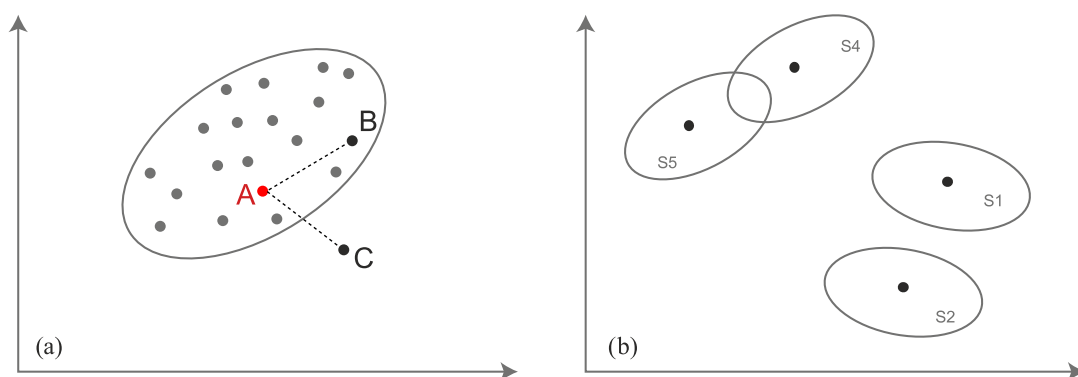


Figure 1: (a) The *Mahalanobis distance* from *A* to *B* is less than from *A* to *C*. However, the Euclidean distances are identical. (b) The *Mahalanobis distance* between the two measurement series *S4* and *S5* is smaller than between *S1* and *S2*. However, the Euclidean distances are identical.

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

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

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

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

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

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

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

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

Summary

A total of 37 534 spectra from 805 different batches for a total of 232 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)	164	297	24 201

From category *A* a total of 24 201 spectra from 297 batches for a total of 164 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)	164	299	12 482

From category *B* a total of 12 482 spectra from 299 batches for a total of 164 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)	216	513	851

From category *C* a total of 851 spectra from 513 batches for a total of 216 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	99	24 010	191	3 944 664
Type B	189	12 152	330	2 034 377
Type C	190	119	549	138 706

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	99.997 68 % (> 99.997 58 %)	99.268 23 % (> 99.252 62 %)
Type B	99.990 98 % (> 99.990 80 %)	97.710 56 % (> 97.680 18 %)
Type C	99.854 01 % (> 99.850 42 %)	14.487 47 % (> 13.843 31 %)

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

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

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

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ba Ji Tian**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60138-2019-09-24
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	G165H0445821	62407	40	from supplier
PhytoComm	Ba Ji Tian	G165H0445821	62408	40	from supplier

Validation samples

A total of 37 534 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 *Ba Ji Tian*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Ba Ji Tian*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ba Ji Tian	G165H0445821	62407 [†]	20
PhytoComm	Ba Ji Tian	G165H0445821	62408 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ba Ji Tian*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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

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

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	80	0	24 121
Type B	0	40	0	12 442
Type C	0	0	0	851

The substance/substance group *Ba Ji 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62408	62408	0.00	11.01
62407	62407	0.00	10.09

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Bai Bian Dou**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60204-2019-09-24
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
PhytoComm	Bai Bian Dou	G093H0510821	62527	40	from supplier
PhytoComm	Bai Bian Dou	G093H0510821	62528	40	from supplier

Validation samples

A total of 37 534 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 *Bai Bian Dou*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Bai Bian Dou*.

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
PhytoComm	Bai Bian Dou	G093H0510821	62527 [†]	20
PhytoComm	Bai Bian Dou	G093H0510821	62528 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Bai Bian Dou*.

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

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

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	7	120	0	12 355
Type C	0	0	2	849

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	99.9289 % (> 99.8984 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62527	62527	0.00	15.51
62210	62210	0.00	6.82
62528	62528	0.00	16.26
62209	62209	0.00	4.72
62195	62195	0.00	15.96
62196	62196	0.00	14.80

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Bai He**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60093-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

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

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 5 spectra from 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Bai He*.

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

- 846 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	5	846

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8208 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well 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	8.51
62138	62138	0.00	8.31

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Bai Hua She She Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60039-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Bai Hua She She Cao; 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
PhytoComm	Bai Hua She She ...	G173HS078RW1	62575	40	from supplier
PhytoComm	Bai Hua She She ...	G173HS078RW1	62576	40	from supplier

Validation samples

A total of 37 534 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 Hua She She Cao*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Bai Hua She She Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Hua She She Cao	G173H1153522	61967 [†]	20
PhytoComm	Bai Hua She She Cao	G173H1153522	61968 [†]	20
PhytoComm	Bai Hua She She Cao	G173HS078RW1	62575 [†]	20
PhytoComm	Bai Hua She She Cao	G173HS078RW1	62576 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 7 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Bai Hua She She Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Bai Hua She She Cao	G173H1153222	3
Phytocomm	Bai Hua She She Cao	G173H1153421	4

- 844 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	7	844

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8201 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62576	62576	0.00	9.63
61967	61967	0.00	19.44
61968	61968	0.00	18.33
62575	62575	0.00	8.48

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Bai Mao Gen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60654-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Bai Mao Gen; Imperatae cylindricae rhizoma

Special notes

When selecting the *Bai Mao 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 *Bai Mao Gen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Bai Mao Gen	G125H0512821	62537	40	from supplier
PhytoComm	Bai Mao Gen	G125H0512821	62538	40	from supplier

Validation samples

A total of 37 534 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 Mao Gen*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Mao Gen	G125H0512821	62537 [†]	20
PhytoComm	Bai Mao Gen	G125H0512821	62538 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Bai Mao Gen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Bai Mao Gen	G125H0512221	2

- 849 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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 Mao 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 *Bai Mao 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	24 121
Type B	0	40	0	12 442
Type C	1	0	2	848

The substance/substance group *Bai Mao 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.8843 % (> 99.2966 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62537	62537	0.00	7.35
62538	62538	0.00	7.06

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Bai Shao Yao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60007-2019-09-24
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	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	G179HS065RQ1	62275	40	from supplier
PhytoComm	Bai Shao Yao	G179HS065RT1	62435	40	from supplier
PhytoComm	Bai Shao Yao	G179HS065RT1	62436	40	from supplier
PhytoComm	Bai Shao Yao	G179HS065RW1	62601	40	from supplier
PhytoComm	Bai Shao Yao	G179HS065RW1	62602	40	from supplier

Validation samples

A total of 37 534 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 *Bai Shao Yao*. These samples are listed above in the [calibration samples](#) section.
- 23 841 spectra from a total of 292 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 239 spectra of 10 reference samples from the substance/substance group *Bai Shao Yao*.

Supplier	Substance	Batch	Sample ID	Spectra
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	G179HS065RQ1	62275 [†]	20
PhytoComm	Bai Shao Yao	G179HS065RQ1	62276	59
PhytoComm	Bai Shao Yao	G179HS065RT1	62435 [†]	20
PhytoComm	Bai Shao Yao	G179HS065RT1	62436 [†]	20
PhytoComm	Bai Shao Yao	G179HS065RW1	62601 [†]	20
PhytoComm	Bai Shao Yao	G179HS065RW1	62602 [†]	20

- 12 243 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 11 spectra from 6 *Apo-Ident* customers from 6 batches from the substance/substance group *Bai Shao Yao*.

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

Supplier	Substance	Batch	Spectra
PhytoComm	Bai Shao Yao	1214401	1
PhytoComm	Bai Shao Yao	G179H0502322	1
Phytocomm	Bai Shao Yao	G179H0502322	1
Phytocomm	Bai Shao Yao	G179H0502121	1
Phytocomm	Bai Shao Yao	g17h0502323	1
Phytocomm	Bai Shao Yao	G179H0502521	5
Phytocomm	Bai Shao Yao	g179h0502322	1

- 840 spectra from 12 *Apo-Ident* customers from a total of 507 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	359	1	23 841
Type B	1	238	1	12 242
Type C	9	8	3	831

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 % (> 99.9687 %)	99.7222 % (> 98.8889 %)
Type B	99.9924 % (> 99.9619 %)	99.5816 % (> 98.3264 %)
Type C	98.6690 % (> 98.0787 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62435	62435	0.00	8.38
61956	61956	0.00	5.81
61955	61955	0.00	5.92
62275	62275	0.00	5.96
62601	62601	0.00	8.30
62602	62602	0.00	7.86
61796	61796	0.00	11.48
61813	61813	0.00	10.45
62436	62436	0.00	7.67

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Bai Xian Pi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60208-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Bai Xian Pi; Dictamni cortex

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	G090HS335RP1	62285	40	from supplier
PhytoComm	Bai Xian Pi	G090HS335RP1	62286	40	from supplier
PhytoComm	Bai Xian Pi	G090HS335RN1	62449	40	from supplier
PhytoComm	Bai Xian Pi	G090HS335RN1	62450	40	from supplier

Validation samples

A total of 37 534 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 Xian Pi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Bai Xian Pi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Xian Pi	G090HS335RP1	62285 [†]	20
PhytoComm	Bai Xian Pi	G090HS335RP1	62286 [†]	20
PhytoComm	Bai Xian Pi	G090HS335RN1	62449 [†]	20
PhytoComm	Bai Xian Pi	G090HS335RN1	62450 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Bai Xian Pi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Bai Xian Pi	G090H0515121	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	1	159	1	24 040
Type B	2	78	2	12 400
Type C	0	0	1	850

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	99.9924 % (> 99.9767 %)	99.3750 % (> 97.5000 %)
Type B	99.9898 % (> 99.9594 %)	97.5000 % (> 93.7500 %)
Type C	100.0000 % (> 98.8311 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62285	62285	0.00	6.67
62449	62449	0.00	6.02
62286	62286	0.00	6.74
62450	62450	0.00	5.44

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Bai Zhu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60015-2019-09-24
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
PhytoComm	Bai Zhu	G041H0501822	62385	40	from supplier
PhytoComm	Bai Zhu	G041H0501822	62386	40	from supplier
PhytoComm	Bai Zhu	G041HS064SG1	62651	40	from supplier
PhytoComm	Bai Zhu	G041HS064SG1	62652	40	from supplier

Validation samples

A total of 37 534 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 Zhu*. These samples are listed above in the [calibration samples](#) section.
- 23 921 spectra from a total of 293 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Zhu	G041H0501621	61837 [†]	20
PhytoComm	Bai Zhu	G041H0501721	62219 [†]	20
PhytoComm	Bai Zhu	G041H0501721	62220 [†]	20
PhytoComm	Bai Zhu	G041H0501822	62385 [†]	20
PhytoComm	Bai Zhu	G041H0501822	62386 [†]	20
PhytoComm	Bai Zhu	G041HS064SG1	62651 [†]	20
PhytoComm	Bai Zhu	G041HS064SG1	62652 [†]	20

- 12 342 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

Supplier	Substance	Batch	Spectra
Phytocomm	Bai Zhu	g041h0501221	3

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

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Supplier	Substance	Batch	Spectra
Phytocomm	Bai Zhu	G041H0501221	1
Phytocomm	Bai Zhu	G041H0501422	3
PhytoComm	Bai Zhu	G041H0501621	1

- 843 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	4	279	1	23 917
Type B	7	136	4	12 335
Type C	2	1	7	841

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	99.9898 % (> 99.9742 %)	99.6429 % (> 98.5714 %)
Type B	99.9644 % (> 99.9339 %)	97.1429 % (> 95.0000 %)
Type C	99.7171 % (> 99.1270 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62386	62386	0.00	5.25

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62219	62219	0.00	3.36
61837	61837	0.00	5.81
62220	62220	0.00	3.98
62385	62385	0.00	4.98
62652	62652	0.00	9.10
62651	62651	0.00	9.47

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Bai Zi Ren**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60197-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Bai Zi Ren; Biotae orientalis 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	G052HS187SK1	62659	40	from supplier
PhytoComm	Bai Zi Ren	G052HS187SK1	62660	40	from supplier

Validation samples

A total of 37 534 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 Zi Ren*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bai Zi Ren	G052HS187SK1	62659 [†]	20
PhytoComm	Bai Zi Ren	G052HS187SK1	62660 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Bai Zi Ren*.

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

- 847 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	37	3	12 442
Type C	0	0	4	847

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	92.5000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62660	62660	0.00	6.20
62659	62659	0.00	6.47

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ban Xia (Jiang)**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60019-2019-09-24
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)	G191HS090QL1	62201	40	from supplier
PhytoComm	Ban Xia (Jiang)	G191HS090QL1	62202	40	from supplier
PhytoComm	Ban Xia (Jiang)	G191HS090SH1	62599	40	from supplier
PhytoComm	Ban Xia (Jiang)	G191HS090SH1	62600	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ban Xia (Jiang)	G191HS090QL1	62201 [†]	20
PhytoComm	Ban Xia (Jiang)	G191HS090QL1	62202 [†]	20
PhytoComm	Ban Xia (Jiang)	G191HS090SH1	62599 [†]	20
PhytoComm	Ban Xia (Jiang)	G191HS090SH1	62600 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Ban Xia (Jiang)*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ban Xia (Jiang)	g191h0526121	1
Phytocomm	Ban Xia (Jiang)	G191H0526322	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	6	159	1	24 035
Type B	9	76	4	12 393
Type C	0	0	2	849

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	99.9784 % (> 99.9628 %)	99.3750 % (> 97.5000 %)
Type B	99.9466 % (> 99.9162 %)	95.0000 % (> 91.2500 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62600	62600	0.00	6.17
62599	62599	0.00	6.22
62201	62201	0.00	4.04
62202	62202	0.00	4.56

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ban Zhi Lian**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60038-2019-09-24
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	G224H0528522	61921	40	from supplier
PhytoComm	Ban Zhi Lian	G224H0528522	61922	40	from supplier

Validation samples

A total of 37 534 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 Zhi Lian*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Ban Zhi Lian*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ban Zhi Lian	G224H0528522	61921 [†]	20
PhytoComm	Ban Zhi Lian	G224H0528522	61922 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Ban Zhi Lian*.

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

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	40	0	12 442
Type C	2	0	4	845

The substance/substance group *Ban Zhi Lian* 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.5370 % (> 98.9478 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61921	61921	0.00	8.60
61922	61922	0.00	8.40

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Bu Gu Zhi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60023-2019-09-24
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
PhytoComm	Bu Gu Zhi	G205H1247822	62487	40	from supplier
PhytoComm	Bu Gu Zhi	G205H1247822	62488	40	from supplier

Validation samples

A total of 37 534 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 *Bu Gu Zhi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Bu Gu Zhi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Bu Gu Zhi	G205H1247621	61939 [†]	20
PhytoComm	Bu Gu Zhi	G205H1247621	61940 [†]	20
PhytoComm	Bu Gu Zhi	G205H1247822	62487 [†]	20
PhytoComm	Bu Gu Zhi	G205H1247822	62488 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 5 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Bu Gu Zhi*.

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

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

- 846 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	1	1	4	845

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.9421 % (> 99.3525 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62487	62487	0.00	18.80
61939	61939	0.00	5.59
62488	62488	0.00	19.12
61940	61940	0.00	5.29

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Cang Er Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60054-2019-09-24
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
PhytoComm	Cang Er Zi	G251H1401821	62503	40	from supplier
PhytoComm	Cang Er Zi	G251H1401821	62504	40	from supplier

Validation samples

A total of 37 534 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 *Cang Er Zi*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Cang Er Zi*.

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
PhytoComm	Cang Er Zi	G251H1401821	62503 [†]	20
PhytoComm	Cang Er Zi	G251H1401821	62504 [†]	20

- 12 362 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Cang Er Zi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Cang Er Zi	G251H1401322	1

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

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Supplier	Substance	Batch	Spectra
Phytocomm	Cang Er Zi	g251h1401021	1
PhytoComm	Cang Er Zi	G251H1401322	1
Phytocomm	Cang Er Zi	G251H1401521	1

- 847 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	1	1	3	846

The substance/substance group *Cang Er 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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	99.5370 % (> 98.9478 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62156	62156	0.00	17.35

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62504	62504	0.00	12.55
61897	61897	0.00	17.23
62503	62503	0.00	12.41
62155	62155	0.00	17.29
61898	61898	0.00	17.13

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Cang Zhu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60160-2019-09-24
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	G042H1402821	62387	40	from supplier
PhytoComm	Cang Zhu	G042H1402821	62388	40	from supplier
PhytoComm	Cang Zhu	G042HS301SG1	62653	40	from supplier
PhytoComm	Cang Zhu	G042HS301SG1	62654	40	from supplier

Validation samples

A total of 37 534 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 Zhu*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Cang Zhu	G042H1402821	62387 [†]	20
PhytoComm	Cang Zhu	G042H1402821	62388 [†]	20
PhytoComm	Cang Zhu	G042HS301SG1	62653 [†]	20
PhytoComm	Cang Zhu	G042HS301SG1	62654 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Cang Zhu*.

Supplier	Substance	Batch	Spectra
Phytocomm	Cang Zhu	g042h1402221	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	1	0	1	849

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.9421 % (> 99.3577 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62387	62387	0.00	7.23
62388	62388	0.00	7.43
62653	62653	0.00	6.36
62654	62654	0.00	6.93

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Chai Hu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60010-2019-09-24
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	G055H1055821	62375	40	from supplier
PhytoComm	Chai Hu	G055H1055821	62376	40	from supplier
PhytoComm	Chai Hu	G055HS233SK1	62661	40	from supplier
PhytoComm	Chai Hu	G055HS233SK1	62662	40	from supplier

Validation samples

A total of 37 534 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 *Chai Hu*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Chai Hu*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chai Hu	G055H1055821	62375 [†]	20
PhytoComm	Chai Hu	G055H1055821	62376 [†]	20
PhytoComm	Chai Hu	G055HS233SK1	62661 [†]	20
PhytoComm	Chai Hu	G055HS233SK1	62662 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 8 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Chai Hu*.

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

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

- 843 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	77	3	12 402
Type C	3	0	8	840

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	96.2500 % (> 92.5000 %)
Type C	99.7145 % (> 99.1244 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62662	62662	0.00	5.30
62661	62661	0.00	6.12
62376	62376	0.00	9.30
62375	62375	0.00	9.14

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Che Qian Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60255-2019-09-24
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	G192HS120SH1	62607	40	from supplier
PhytoComm	Che Qian Zi	G192HS120SH1	62608	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Che Qian Zi	G192HS120SH1	62607 [†]	20
PhytoComm	Che Qian Zi	G192HS120SH1	62608 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 6 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Che Qian Zi*.

Supplier	Substance	Batch	Spectra
PhytoComm	Che Qian Zi	G192H0723321	2
Phytocomm	Che Qian Zi	410704805	1
Phytocomm	Che Qian Zi	G192H0723421	2
PhytoComm	Che Qian Zi	G192H0723621	1

- 845 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	79	1	24 121
Type B	0	40	0	12 442
Type C	0	0	6	845

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 % (> 99.9689 %)	98.7500 % (> 95.0000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8204 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62607	62607	0.00	6.06
62608	62608	0.00	5.71

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Chen Pi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60009-2019-09-24
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	G073H1128821	62377	40	from supplier
PhytoComm	Chen Pi	G073H1128821	62378	40	from supplier
PhytoComm	Chen Pi	G073HS254RR1	62445	40	from supplier
PhytoComm	Chen Pi	G073HS254RR1	62446	40	from supplier
PhytoComm	Chen Pi	G073HS254SG1	62669	40	from supplier
PhytoComm	Chen Pi	G073HS254SG1	62670	40	from supplier

Validation samples

A total of 37 534 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 *Chen Pi*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Chen Pi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chen Pi	G073H1128821	62377 [†]	20
PhytoComm	Chen Pi	G073H1128821	62378 [†]	20
PhytoComm	Chen Pi	G073HS254RR1	62445 [†]	20
PhytoComm	Chen Pi	G073HS254RR1	62446 [†]	20
PhytoComm	Chen Pi	G073HS254SG1	62669 [†]	20
PhytoComm	Chen Pi	G073HS254SG1	62670 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Chen Pi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Chen Pi	G073H1128222	1

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

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Supplier	Substance	Batch	Spectra
PhytoComm	Chen Pi	G073H1128222	1
Phytocomm	Chen Pi	g07h1128221	1
Phytocomm	Chen Pi	g073h1128222	1

- 847 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	0	4	847

The substance/substance group *Chen 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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62377	62377	0.00	9.37
62445	62445	0.00	7.63

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62669	62669	0.00	7.40
62446	62446	0.00	8.14
62378	62378	0.00	10.50
62670	62670	0.00	7.39

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Chi Shao (Yao)**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60014-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Chi Shao (Yao); Paeoniae radix rubra

Special notes

When selecting the *Chi 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 *Chi Shao (Yao)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Chi Shao (Yao)	G180H0705821	62363	40	from supplier
PhytoComm	Chi Shao (Yao)	G180H0705821	62364	40	from supplier
PhytoComm	Chi Shao (Yao)	G180H0705822	62481	40	from supplier
PhytoComm	Chi Shao (Yao)	G180H0705822	62482	40	from supplier

Validation samples

A total of 37 534 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 *Chi Shao (Yao)*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Chi Shao (Yao)*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chi Shao (Yao)	G180H0705821	62363 [†]	20
PhytoComm	Chi Shao (Yao)	G180H0705821	62364 [†]	20
PhytoComm	Chi Shao (Yao)	G180H0705822	62481 [†]	20
PhytoComm	Chi Shao (Yao)	G180H0705822	62482 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Chi Shao (Yao)*.

Supplier	Substance	Batch	Spectra
Phytocomm	Chi Shao (Yao)	G180H0705321	1
Phytocomm	Chi Shao (Yao)	g180h0705122	1
Phytocomm	Chi Shao (Yao)	G189H0705321	1
Phytocomm	Chi Shao (Yao)	G180H0705422	1

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

- 847 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Chi 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 *Chi 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	2	2	847

The substance/substance group *Chi Shao (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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62482	62482	0.00	13.41
62364	62364	0.00	11.40
62363	62363	0.00	12.00
62481	62481	0.00	13.22

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Chuan Lian Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60078-2019-09-24
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	G157H0306821	62355	40	from supplier
PhytoComm	Chuan Lian Zi	G157H0306821	62356	40	from supplier

Validation samples

A total of 37 534 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 Lian Zi*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chuan Lian Zi	G157H0306821	62355 [†]	20
PhytoComm	Chuan Lian Zi	G157H0306821	62356 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 3 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Chuan Lian Zi*.

Supplier	Substance	Batch	Spectra
PhytoComm	Chuan Lian Zi	G157H0306421	1
PhytoComm	Chuan Lian Zi	G157H0306421	2

- 848 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	40	0	12 442
Type C	3	0	3	845

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.7222 % (> 99.1335 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62355	62355	0.00	9.48
62356	62356	0.00	11.33

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Chuan Xiong**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60013-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Chuan Xiong; 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
PhytoComm	Chuan Xiong	G136H0305622	62291	40	from supplier
PhytoComm	Chuan Xiong	G136H0305622	62292	40	from supplier
PhytoComm	Chuan Xiong	G136HS031RR2	62457	40	from supplier
PhytoComm	Chuan Xiong	G136HS031RR2	62458	40	from supplier
PhytoComm	Chuan Xiong	G136HS031SH1	62689	40	from supplier
PhytoComm	Chuan Xiong	G136HS031SH1	62690	40	from supplier

Validation samples

A total of 37 534 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 8 reference samples from the substance/substance group *Chuan Xiong*. These samples are listed above in the [calibration samples](#) section.
- 23 881 spectra from a total of 293 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 160 spectra of 8 reference samples from the substance/substance group *Chuan Xiong*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chuan Xiong	G136H0305621	61975 [†]	20
PhytoComm	Chuan Xiong	G136H0305621	61976 [†]	20
PhytoComm	Chuan Xiong	G136H0305622	62291 [†]	20
PhytoComm	Chuan Xiong	G136H0305622	62292 [†]	20
PhytoComm	Chuan Xiong	G136HS031RR2	62457 [†]	20
PhytoComm	Chuan Xiong	G136HS031RR2	62458 [†]	20
PhytoComm	Chuan Xiong	G136HS031SH1	62689 [†]	20
PhytoComm	Chuan Xiong	G136HS031SH1	62690 [†]	20

- 12 322 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 6 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Chuan Xiong*.

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

Supplier	Substance	Batch	Spectra
PhytoComm	Chuan Xiong	G136H0305221	2
Phytocomm	Chuan Xiong	G136H0305221	1
Phytocomm	Chuan Xiong	g136h0305121	1
Phytocomm	Chuan Xiong	G136H0305421	2

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	320	0	23 881
Type B	1	157	3	12 321
Type C	3	1	5	842

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 % (> 99.9687 %)	100.0000 % (> 98.1250 %)
Type B	99.9924 % (> 99.9619 %)	98.1250 % (> 96.2500 %)
Type C	99.8457 % (> 99.2559 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62457	62457	0.00	7.38

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61975	61975	0.00	8.08
62690	62690	0.00	4.63
62292	62292	0.00	7.67
62291	62291	0.00	7.55
62458	62458	0.00	7.16
62689	62689	0.00	5.32
61976	61976	0.00	8.42

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Chuang Mu Xiang**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50323-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Chuang Mu Xiang; Vladimira radix

Special notes

When selecting the *Chuang Mu 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 *Chuang Mu Xiang*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Chuang Mu Xiang	G219HS046SK1	62643	40	from supplier
PhytoComm	Chuang Mu Xiang	G219HS046SK1	62644	40	from supplier

Validation samples

A total of 37 534 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 *Chuang Mu Xiang*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Chuang Mu Xiang*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Chuang Mu Xiang	G219HS046SK1	62643 [†]	20
PhytoComm	Chuang Mu Xiang	G219HS046SK1	62644 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 5 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Chuang Mu Xiang*.

Supplier	Substance	Batch	Spectra
Phytocomm	Chuang Mu Xiang	G219H0309322	1
Phytocomm	Chuang Mu Xiang	g219h0309321	1
Phytocomm	Chuang Mu Xiang	g219h0309322	1
Phytocomm	Chuang Mu Xiang	G219H0309521	2

- 846 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 sub-

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

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

Validation results

The validation runs checked whether the substance/substance group *Chuang Mu 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 *Chuang Mu 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	24 121
Type B	0	40	0	12 442
Type C	0	0	5	846

The substance/substance group *Chuang Mu 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8208 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62643	62643	0.00	9.81
62644	62644	0.00	9.88

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ci Wu Jia**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60354-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ci Wu Jia; 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	G302HS422SH1	62623	40	from supplier
PhytoComm	Ci Wu Jia	G302HS422SH1	62624	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ci Wu Jia	G302HS422SH1	62623 [†]	20
PhytoComm	Ci Wu Jia	G302HS422SH1	62624 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ci Wu Jia*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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

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

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	76	4	24 121
Type B	0	35	5	12 442
Type C	0	0	0	851

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	95.0000 % (> 91.2500 %)
Type B	100.0000 % (> 99.9394 %)	87.5000 % (> 80.0000 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62623	62623	0.00	3.22
62624	62624	0.00	2.92

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Da Huang**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60140-2019-09-24
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
PhytoComm	Da Huang	G212H0320822	62495	40	from supplier
PhytoComm	Da Huang	G212H0320822	62496	40	from supplier

Validation samples

A total of 37 534 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 *Da Huang*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Da Huang*.

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
PhytoComm	Da Huang	G212H0320822	62495 [†]	20
PhytoComm	Da Huang	G212H0320822	62496 [†]	20

- 12 362 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 7 spectra from 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Da Huang*.

Supplier	Substance	Batch	Spectra
Phytocomm	Da Huang	G212H0320321	2

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

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

- 844 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	5	2	844

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8201 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well 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	37.04
62158	62158	0.00	35.09

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62157	62157	0.00	35.02
62496	62496	0.00	36.80
62130	62130	0.00	37.03
62495	62495	0.00	36.83

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Da Zao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60055-2019-09-24
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	G129H0316621	62215	40	from supplier
PhytoComm	Da Zao	G129H0316621	62216	40	from supplier
PhytoComm	Da Zao	G129HS019RT1	62455	40	from supplier
PhytoComm	Da Zao	G129HS019RT1	62456	40	from supplier
PhytoComm	Da Zao	G129H0316821	62539	40	from supplier
PhytoComm	Da Zao	G129H0316821	62540	40	from supplier

Validation samples

A total of 37 534 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 *Da Zao*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Da Zao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Da Zao	G129H0316621	62215 [†]	20
PhytoComm	Da Zao	G129H0316621	62216 [†]	20
PhytoComm	Da Zao	G129HS019RT1	62455 [†]	20
PhytoComm	Da Zao	G129HS019RT1	62456 [†]	20
PhytoComm	Da Zao	G129H0316821	62539 [†]	20
PhytoComm	Da Zao	G129H0316821	62540 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Da Zao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Da Zao	g129h0316221	1
Phytocomm	Da Zao	G129H0316521	3

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

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	4	0	847

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62456	62456	0.00	11.00
62540	62540	0.00	14.85
62539	62539	0.00	15.09
62215	62215	0.00	15.13
62216	62216	0.00	15.22
62455	62455	0.00	11.34

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Dan Dou Chi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60794-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 041 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

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

- 12 407 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Dan Dou Chi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Dan Dou Chi	G232HS239	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 041
Type B	0	75	0	12 407
Type C	0	0	1	850

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9392 %)	100.0000 % (> 92.0000 %)
Type C	100.0000 % (> 98.8311 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62174	62174	0.00	56.61
62173	62173	0.00	56.89
61909	61909	0.00	45.64
61910	61910	0.00	47.68

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Dan Shen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60030-2019-09-24
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	G214H0441821	62309	40	from supplier
PhytoComm	Dan Shen	G214H0441821	62310	40	from supplier
PhytoComm	Dan Shen	G214HS059SG1	62573	40	from supplier
PhytoComm	Dan Shen	G214HS059SG1	62574	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Dan Shen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dan Shen	G214H0441821	62309 [†]	20
PhytoComm	Dan Shen	G214H0441821	62310 [†]	20
PhytoComm	Dan Shen	G214HS059SG1	62573 [†]	20
PhytoComm	Dan Shen	G214HS059SG1	62574 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 9 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Dan Shen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Dan Shen	G214H0441121	1
PhytoComm	Dan Shen	G214H0441221	2
Phytocomm	Dan Shen	G214H0441221	1
Phytocomm	Dan Shen	G214H0441322	1
PhytoComm	Dan Shen	G214H0441322	1
Phytocomm	Dan Shen	g214h0441121	1
PhytoComm	Dan Shen	G214H0441522	1
Phytocomm	Dan Shen	G214H0441522	1

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

- 842 spectra from 12 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	159	1	24 041
Type B	4	80	0	12 398
Type C	3	0	9	839

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 % (> 99.9687 %)	99.3750 % (> 97.5000 %)
Type B	99.9619 % (> 99.9315 %)	100.0000 % (> 92.5000 %)
Type C	99.4599 % (> 98.8697 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62309	62309	0.00	11.34
62310	62310	0.00	11.21
62573	62573	0.00	4.26
62574	62574	0.00	7.42

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Dan Zhu Ye**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60147-2019-09-24
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
PhytoComm	Dan Zhu Ye	G046H1105821	62581	40	from supplier
PhytoComm	Dan Zhu Ye	G046H1105821	62582	40	from supplier

Validation samples

A total of 37 534 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 Zhu Ye*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Dan Zhu Ye*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dan Zhu Ye	G046H1105621	62105 [†]	20
PhytoComm	Dan Zhu Ye	G046H1105621	62106 [†]	20
PhytoComm	Dan Zhu Ye	G046H1105821	62581 [†]	20
PhytoComm	Dan Zhu Ye	G046H1105821	62582 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Dan Zhu Ye*.

Supplier	Substance	Batch	Spectra
Phytocomm	Dan Zhu Ye	G046H1105321	2

- 849 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	158	2	24 041
Type B	1	78	2	12 401
Type C	10	0	2	839

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 % (> 99.9687 %)	98.7500 % (> 96.8750 %)
Type B	99.9848 % (> 99.9543 %)	97.5000 % (> 93.7500 %)
Type C	98.4375 % (> 97.8498 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62106	62106	0.00	6.63
62582	62582	0.00	10.02
62105	62105	0.00	5.17
62581	62581	0.00	9.90

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Dang Gui**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60003-2019-09-24
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	G022H1306822	62413	40	from supplier
PhytoComm	Dang Gui	G022H1306822	62414	40	from supplier
PhytoComm	Dang Gui	G022HS290SK1	62649	40	from supplier
PhytoComm	Dang Gui	G022HS290SK1	62650	40	from supplier

Validation samples

A total of 37 534 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 *Dang Gui*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Dang Gui*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dang Gui	G022H1306822	62413 [†]	20
PhytoComm	Dang Gui	G022H1306822	62414 [†]	20
PhytoComm	Dang Gui	G022HS290SK1	62649 [†]	20
PhytoComm	Dang Gui	G022HS290SK1	62650 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 12 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Dang Gui*.

Supplier	Substance	Batch	Spectra
PhytoComm	Dang Gui	G13-0784	1
PhytoComm	Dang Gui	G022H1306121	1
Phytocomm	Dang Gui	g022h1306121	3
Phytocomm	Dang Gui	G022H1306422	3
PhytoComm	Dang Gui	G022H1306621	4

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

- 839 spectra from 12 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	79	1	12 402
Type C	1	2	10	838

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	98.7500 % (> 95.0000 %)
Type C	99.9228 % (> 99.3325 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62414	62414	0.00	5.32
62649	62649	0.00	8.36
62650	62650	0.00	8.20
62413	62413	0.00	6.11

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Dang Gui Wei**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60308-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dang Gui Wei; Angelicae sinensis radix extremas

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
PhytoComm	Dang Gui Wei	G312HS291SK1	62621	40	from supplier
PhytoComm	Dang Gui Wei	G312HS291SK1	62622	40	from supplier

Validation samples

A total of 37 534 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 *Dang Gui Wei*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Dang Gui Wei*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dang Gui Wei	G312H1307621	61885 [†]	20
PhytoComm	Dang Gui Wei	G312H1307621	61886 [†]	20
PhytoComm	Dang Gui Wei	G312HS291SK1	62621 [†]	20
PhytoComm	Dang Gui Wei	G312HS291SK1	62622 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Dang Gui Wei*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

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

Validation results

The validation runs checked whether the substance/substance group *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	160	0	24 041
Type B	0	80	0	12 402
Type C	7	0	0	844

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.2333 % (> 98.6424 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62622	62622	0.00	7.98
61885	61885	0.00	6.47
62621	62621	0.00	7.65
61886	61886	0.00	6.46

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Dang Shen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60000-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dang Shen; Codonopsis pilosulae radix

Special notes

When selecting the *Dang 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 *Dang Shen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Dang Shen	G077H2001821	62367	40	from supplier
PhytoComm	Dang Shen	G077H2001821	62368	40	from supplier
PhytoComm	Dang Shen	G077HS352RQ1	62369	40	from supplier
PhytoComm	Dang Shen	G077HS352RQ1	62370	40	from supplier
PhytoComm	Dang Shen	G077HS352SG1	62673	40	from supplier
PhytoComm	Dang Shen	G077HS352SG1	62674	40	from supplier

Validation samples

A total of 37 534 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 *Dang Shen*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Dang Shen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dang Shen	G077H2001821	62367 [†]	20
PhytoComm	Dang Shen	G077H2001821	62368 [†]	20
PhytoComm	Dang Shen	G077HS352RQ1	62369 [†]	20
PhytoComm	Dang Shen	G077HS352RQ1	62370 [†]	20
PhytoComm	Dang Shen	G077HS352SG1	62673 [†]	20
PhytoComm	Dang Shen	G077HS352SG1	62674 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

Supplier	Substance	Batch	Spectra
Phytocomm	Dang Shen	G077H2001022	1

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Dang Shen	g077h2001222	2
PhytoComm	Dang Shen	G077H2001521	2
PhytoComm	Dang Shen	G077H2001521	2
PhytoComm	Dang Shen	G077H2001621	1

- 843 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 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 *Dang 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	240	0	23 961
Type B	1	117	3	12 361
Type C	1	4	4	842

The substance/substance group *Dang 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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	99.9848 % (> 99.9543 %)	97.5000 % (> 95.0000 %)
Type C	99.8843 % (> 99.2942 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62367	62367	0.00	10.28
62673	62673	0.00	6.45
62368	62368	0.00	10.32
62370	62370	0.00	8.29
62674	62674	0.00	6.25
62369	62369	0.00	8.19

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Di Gu Pi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60036-2019-09-24
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
PhytoComm	Di Gu Pi	G149H0601821	62347	40	from supplier
PhytoComm	Di Gu Pi	G149H0601821	62348	40	from supplier
PhytoComm	Di Gu Pi	G149HS101SK1	62691	40	from supplier
PhytoComm	Di Gu Pi	G149HS101SK1	62692	40	from supplier

Validation samples

A total of 37 534 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 *Di Gu Pi*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Di Gu Pi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Di Gu Pi	G149H0601622	62211 [†]	20
PhytoComm	Di Gu Pi	G149H0601622	62212 [†]	20
PhytoComm	Di Gu Pi	G149H0601821	62347 [†]	20
PhytoComm	Di Gu Pi	G149H0601821	62348 [†]	20
PhytoComm	Di Gu Pi	G149HS101SK1	62691 [†]	20
PhytoComm	Di Gu Pi	G149HS101SK1	62692 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Di Gu Pi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Di Gu Pi	g149h060112	1
Phytocomm	Di Gu Pi	G149H0601421	1
PhytoComm	Di Gu Pi	G149H0601421	2

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

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	1	238	2	23 960
Type B	2	113	7	12 360
Type C	5	0	4	842

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	99.9962 % (> 99.9805 %)	99.1667 % (> 97.9167 %)
Type B	99.9848 % (> 99.9543 %)	94.1667 % (> 91.6667 %)
Type C	99.6348 % (> 99.0455 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62212	62212	0.00	10.85
62347	62347	0.00	9.11
62211	62211	0.00	10.35
62691	62691	0.00	4.16
62692	62692	0.00	3.92
62348	62348	0.00	9.36

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Dong Gua Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60202-2019-09-24
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	G049H0551822	62513	40	from supplier
PhytoComm	Dong Gua Zi	G049H0551822	62514	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Dong Gua Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dong Gua Zi	G049H0551822	62513 [†]	20
PhytoComm	Dong Gua Zi	G049H0551822	62514 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Dong Gua Zi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Dong Gua Zi	G049H0551221	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	1	850

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8311 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62514	62514	0.00	20.14
62513	62513	0.00	19.91

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Dong Kui Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60483-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dong Kui Zi; Abutili 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	G001H0834821	62505	40	from supplier
PhytoComm	Dong Kui Zi	G001H0834821	62506	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Dong Kui Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Dong Kui Zi	G001H0834821	62505 [†]	20
PhytoComm	Dong Kui Zi	G001H0834821	62506 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Dong Kui Zi*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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

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

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	24 121
Type B	0	40	0	12 442
Type C	0	0	0	851

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62505	62505	0.00	18.78
62506	62506	0.00	19.10

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Du Huo**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50259-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Du Huo; Angelicae pubescentis radix

Special notes

When selecting the *Du 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 *Du Huo*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Du Huo	G021H1610821	62391	40	from supplier
PhytoComm	Du Huo	G021H1610821	62392	40	from supplier

Validation samples

A total of 37 534 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 *Du Huo*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Du Huo*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Du Huo	G021H1610821	62391 [†]	20
PhytoComm	Du Huo	G021H1610821	62392 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 3 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Du Huo*.

Supplier	Substance	Batch	Spectra
Phytocomm	Du Huo	g021h610221	1
Phytocomm	Du Huo	G021H1610421	2

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

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

Validation results

The validation runs checked whether the substance/substance group *Du 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 *Du 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	24 121
Type B	0	40	0	12 442
Type C	1	0	3	847

The substance/substance group *Du 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.9228 % (> 99.3341 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62392	62392	0.00	9.80
62391	62391	0.00	9.82

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Du Zhong**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60214-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Du Zhong; Eucommiae ulmoidis cortex

Special notes

When selecting the *Du Zhong* substance/substance group, the following information is displayed to 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 *Du Zhong*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Du Zhong	G101H0736821	62335	40	from supplier
PhytoComm	Du Zhong	G101H0736821	62336	40	from supplier
PhytoComm	Du Zhong	G101HS133SH1	62579	40	from supplier
PhytoComm	Du Zhong	G101HS133SH1	62580	40	from supplier

Validation samples

A total of 37 534 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 *Du Zhong*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Du Zhong*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Du Zhong	G101H0736821	62335 [†]	20
PhytoComm	Du Zhong	G101H0736821	62336 [†]	20
PhytoComm	Du Zhong	G101HS133SH1	62579 [†]	20
PhytoComm	Du Zhong	G101HS133SH1	62580 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 8 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Du Zhong*.

Supplier	Substance	Batch	Spectra
Phytocomm	Du Zhong	G101H0736321	1
Phytocomm	Du Zhong	g101h076521	1
Phytocomm	Du Zhong	g101h0736021	1
Phytocomm	Du Zhong	G101H0736522	5

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

- 843 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Du Zhong* 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 *Du Zhong* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according 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	158	2	24 040
Type B	0	69	11	12 402
Type C	0	0	8	843

The substance/substance group *Du Zhong* 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	99.9962 % (> 99.9806 %)	98.7500 % (> 96.8750 %)
Type B	100.0000 % (> 99.9391 %)	86.2500 % (> 82.5000 %)
Type C	100.0000 % (> 98.8198 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62335	62335	0.00	4.15
62579	62579	0.00	4.83
62580	62580	0.00	4.83
62336	62336	0.00	3.87

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **E Zhu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50344-2019-09-24
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	G083H1110821	62515	40	from supplier
PhytoComm	E Zhu	G083H1110821	62516	40	from supplier

Validation samples

A total of 37 534 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 *E Zhu*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	E Zhu	G083H1110821	62515 [†]	20
PhytoComm	E Zhu	G083H1110821	62516 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *E Zhu*.

Supplier	Substance	Batch	Spectra
Phytocomm	E Zhu	H1110021	1
Phytocomm	E Zhu	h1110021	1
PhytoComm	E Zhu	G083H1110222	2

- 847 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	40	0	12 442
Type C	0	0	4	847

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62516	62516	0.00	17.28
62515	62515	0.00	16.74

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Fang Feng**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50261-2019-09-24
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	G217H0728821	62307	40	from supplier
PhytoComm	Fang Feng	G217H0728821	62308	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Fang Feng*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fang Feng	G217H0728821	62307 [†]	20
PhytoComm	Fang Feng	G217H0728821	62308 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 7 spectra from 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Fang Feng*.

Supplier	Substance	Batch	Spectra
Phytocomm	Fang Feng	g217h0728923	1
Phytocomm	Fang Feng	g217h0728221	1
Phytocomm	Fang Feng	G217H0728521	3
PhytoComm	Fang Feng	G217H0728521	2

- 844 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	2	0	7	842

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.7685 % (> 99.1785 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62307	62307	0.00	9.37
62308	62308	0.00	10.21

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Fang Ji**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60270-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Fang Ji*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fang Ji	G236HS122QM1	62179 [†]	20
PhytoComm	Fang Ji	G236HS122QM1	62180 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Fang Ji*.

Supplier	Substance	Batch	Spectra
Phytocomm	Fang Ji	G236H0727321	1
PhytoComm	Fang Ji	G236H0727123	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	2	849

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well 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	5.16
62180	62180	0.00	5.07

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Fo Shou**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60119-2019-09-24
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	G307HS159RQ1	62419	40	from supplier
PhytoComm	Fo Shou	G307HS159RQ1	62420	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Fo Shou*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fo Shou	G307HS159RQ1	62419 [†]	20
PhytoComm	Fo Shou	G307HS159RQ1	62420 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Fo Shou*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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

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

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	79	1	24 121
Type B	0	39	1	12 442
Type C	0	0	0	851

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 % (> 99.9689 %)	98.7500 % (> 95.0000 %)
Type B	100.0000 % (> 99.9394 %)	97.5000 % (> 90.0000 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62419	62419	0.00	6.91
62420	62420	0.00	4.85

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Fu Ling**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50260-2019-09-24
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	G200HS211RT1	62429	40	from supplier
PhytoComm	Fu Ling	G200HS211RT1	62430	40	from supplier
PhytoComm	Fu Ling	G200HS211SH1	62597	40	from supplier
PhytoComm	Fu Ling	G200HS211SH1	62598	40	from supplier

Validation samples

A total of 37 534 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 *Fu Ling*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Fu Ling*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fu Ling	G200HS211RT1	62429 [†]	20
PhytoComm	Fu Ling	G200HS211RT1	62430 [†]	20
PhytoComm	Fu Ling	G200HS211SH1	62597 [†]	20
PhytoComm	Fu Ling	G200HS211SH1	62598 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 12 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Fu Ling*.

Supplier	Substance	Batch	Spectra
Phytocomm	Fu Ling	G200H1019221	1
Phytocomm	Fu Ling	G200H1019321	1
Phytocomm	Fu Ling	g200h1019321	3
PhytoComm	Fu Ling	G200H1019221	1
PhytoComm	Fu Ling	G200H1019321	1
Phyto Comm	Fu Ling	G200H1019522	1

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
Phytocomm	Fu Ling	G200H1019522	2
PhytoComm	Fu Ling	G200H1019522	1
PhytoComm	Fu Ling	G200H1019622	1

- 839 spectra from 11 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	12	839

The substance/substance group *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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8193 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62598	62598	0.00	8.57
62430	62430	0.00	8.78
62597	62597	0.00	9.29
62429	62429	0.00	9.29

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Fu Shen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60004-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Fu Shen; Poriae cocos sclerotium paradicis

Special notes

When selecting the *Fu 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 *Fu Shen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Fu Shen	G201HS212SH1	62617	40	from supplier
PhytoComm	Fu Shen	G201HS212SH1	62618	40	from supplier

Validation samples

A total of 37 534 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 Shen*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Fu Shen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fu Shen	G201HS212SH1	62617 [†]	20
PhytoComm	Fu Shen	G201HS212SH1	62618 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Fu Shen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Fu Shen	g201h1021321	1
Phytocomm	Fu Shen	G201H1021321	1
Phytocomm	Fu Shen	G201H1021422	2

- 847 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 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 *Fu 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	24 121
Type B	0	40	0	12 442
Type C	1	0	4	846

The substance/substance group *Fu 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.8843 % (> 99.2950 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62617	62617	0.00	7.51
62618	62618	0.00	6.99

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Fu Xiao Mai**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60081-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Fu Xiao Mai; Triticum aestivum 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
PhytoComm	Fu Xiao Mai	G244HS021RT1	62423	40	from supplier
PhytoComm	Fu Xiao Mai	G244HS021RT1	62424	40	from supplier
PhytoComm	Fu Xiao Mai	G244HS021SK1	62631	40	from supplier
PhytoComm	Fu Xiao Mai	G244HS021SK1	62632	40	from supplier

Validation samples

A total of 37 534 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 *Fu Xiao Mai*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Fu Xiao Mai*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fu Xiao Mai	G244HS021QM1	62183 [†]	20
PhytoComm	Fu Xiao Mai	G244HS021QM1	62184 [†]	20
PhytoComm	Fu Xiao Mai	G244HS021RT1	62423 [†]	20
PhytoComm	Fu Xiao Mai	G244HS021RT1	62424 [†]	20
PhytoComm	Fu Xiao Mai	G244HS021SK1	62631 [†]	20
PhytoComm	Fu Xiao Mai	G244HS021SK1	62632 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Fu Xiao Mai*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

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

Validation results

The validation runs checked whether the substance/substance group *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	10	223	17	23 951
Type B	23	106	14	12 339
Type C	0	0	0	851

The substance/substance group *Fu Xiao Mai* 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	99.9708 % (> 99.9551 %)	92.9167 % (> 91.6667 %)
Type B	99.8552 % (> 99.8247 %)	88.3333 % (> 85.8333 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62424	62424	0.00	2.86
62184	62184	0.00	2.85
62423	62423	0.00	4.22
62183	62183	0.00	3.08
62631	62631	0.00	4.52
62632	62632	0.00	2.76

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Fu Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50884-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Fu Zi; 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	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 37 534 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 *Fu Zi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Fu Zi	G005H0801624	62081 [†]	20
PhytoComm	Fu Zi	G005H0801624	62082 [†]	20
PhytoComm	Fu Zi	G005H0801723	62225 [†]	20
PhytoComm	Fu Zi	G005H0801723	62226 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Fu Zi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Fu Zi	g005h0801122	1
Phytocomm	Fu Zi	G005H0801322	1
phytocomm	Fu Zi	g005h0801322	1
Phytocomm	Fu Zi	G005H0801524	1

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

- 847 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	73	7	12 402
Type C	1	0	4	846

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	91.2500 % (> 87.5000 %)
Type C	99.8843 % (> 99.2950 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62226	62226	0.00	8.78
62081	62081	0.00	6.72
62082	62082	0.00	6.16
62225	62225	0.00	9.38

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Gan Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60011-2019-09-24
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
PhytoComm	Gan Cao	G119H0521822	62341	40	from supplier
PhytoComm	Gan Cao	G119H0521822	62342	40	from supplier
PhytoComm	Gan Cao	G119H0521823	62533	40	from supplier
PhytoComm	Gan Cao	G119H0521823	62534	40	from supplier

Validation samples

A total of 37 534 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 *Gan Cao*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Gan Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gan Cao	G119H0521622	62145 [†]	20
PhytoComm	Gan Cao	G119H0521622	62146 [†]	20
PhytoComm	Gan Cao	G119H0521822	62341 [†]	20
PhytoComm	Gan Cao	G119H0521822	62342 [†]	20
PhytoComm	Gan Cao	G119H0521823	62533 [†]	20
PhytoComm	Gan Cao	G119H0521823	62534 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 15 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Gan Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Gan Cao	g119h0521121	1

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

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Supplier	Substance	Batch	Spectra
Phytocomm	Gan Cao	G119H0521121	1
PhytoComm	Gan Cao	G119H0521121	4
Phytocomm	Gan Cao	G119H0521522	8
PhytoComm	Gan Cao	G119H0521524	1

- 836 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	9	6	836

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8191 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62341	62341	0.00	19.95

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62146	62146	0.00	7.96
62534	62534	0.00	18.00
62342	62342	0.00	19.34
62533	62533	0.00	19.27
62145	62145	0.00	8.25

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Gan Jiang**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60077-2019-09-24
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	G252H1145821	62325	40	from supplier
PhytoComm	Gan Jiang	G252H1145821	62326	40	from supplier

Validation samples

A total of 37 534 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 Jiang*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Gan Jiang*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gan Jiang	G252H1145821	62325 [†]	20
PhytoComm	Gan Jiang	G252H1145821	62326 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Gan Jiang*.

Supplier	Substance	Batch	Spectra
Phytocomm	Gan Jiang	G252H1145221	1
Phytocomm	Gan Jiang	g252h01145221	1
Phytocomm	Gan Jiang	G252H1145421	1
Phytocomm	Gan Jiang	G252H1145521	1

- 847 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	40	0	12 442
Type C	2	1	3	845

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.4213 % (> 98.8320 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62325	62325	0.00	11.15
62326	62326	0.00	11.53

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ge Gen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60050-2019-09-24
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
PhytoComm	Ge Gen	G206H1301822	62489	40	from supplier
PhytoComm	Ge Gen	G206H1301822	62490	40	from supplier

Validation samples

A total of 37 534 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 *Ge Gen*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Ge Gen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ge Gen	G206H1301621	61949 [†]	20
PhytoComm	Ge Gen	G206H1301621	61950 [†]	20
PhytoComm	Ge Gen	G206H1301822	62489 [†]	20
PhytoComm	Ge Gen	G206H1301822	62490 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 5 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Ge Gen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ge Gen	G206H1301221	2
PhytoComm	Ge Gen	G206H1301323	1
Phytocomm	Ge Gen	G206H1301422	2

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

- 846 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	5	846

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8208 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61950	61950	0.00	25.24
62490	62490	0.00	23.98
61949	61949	0.00	23.56
62489	62489	0.00	23.98

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Gou Qi Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60094-2019-09-24
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	G150H0913821	62349	40	from supplier
PhytoComm	Gou Qi Zi	G150H0913821	62350	40	from supplier
PhytoComm	Gou Qi Zi	G150HS171SK1	62615	40	from supplier
PhytoComm	Gou Qi Zi	G150HS171SK1	62616	40	from supplier

Validation samples

A total of 37 534 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 *Gou Qi Zi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Gou Qi Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gou Qi Zi	G150H0913821	62349 [†]	20
PhytoComm	Gou Qi Zi	G150H0913821	62350 [†]	20
PhytoComm	Gou Qi Zi	G150HS171SK1	62615 [†]	20
PhytoComm	Gou Qi Zi	G150HS171SK1	62616 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 6 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Gou Qi Zi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Gou Qi Zi	g150h0913221	1
PhytoComm	Gou Qi Zi	G150H0913221	1
Phytocomm	Gou Qi Zi	G150H0913422	4

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

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	7	2	4	838

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.2196 % (> 98.6298 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62616	62616	0.00	9.30
62350	62350	0.00	6.57
62615	62615	0.00	9.94
62349	62349	0.00	7.68

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Gou Teng**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60097-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Gou Teng; Uncariae ramulus cum uncis

Special notes

When selecting the *Gou 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 *Gou Teng*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gou Teng	G247H1210822	62313	40	from supplier
PhytoComm	Gou Teng	G247H1210822	62314	40	from supplier
PhytoComm	Gou Teng	G247HS288SG1	62629	40	from supplier
PhytoComm	Gou Teng	G247HS288SG1	62630	40	from supplier

Validation samples

A total of 37 534 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 *Gou Teng*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Gou Teng*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gou Teng	G247H1210822	62313 [†]	20
PhytoComm	Gou Teng	G247H1210822	62314 [†]	20
PhytoComm	Gou Teng	G247HS288SG1	62629 [†]	20
PhytoComm	Gou Teng	G247HS288SG1	62630 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 3 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Gou Teng*.

Supplier	Substance	Batch	Spectra
Phytocomm	Gou Teng	g247h1210122	1
Phytocomm	Gou Teng	G247H1210422	2

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 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 *Gou 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	159	1	24 041
Type B	0	76	4	12 402
Type C	2	0	3	846

The substance/substance group *Gou Teng* 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 % (> 99.9687 %)	99.3750 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	95.0000 % (> 91.2500 %)
Type C	99.5370 % (> 98.9483 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62314	62314	0.00	20.06
62313	62313	0.00	19.14
62629	62629	0.00	5.66
62630	62630	0.00	2.96

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Gua Lou**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60128-2019-09-24
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	G241H1096523	61787	40	from supplier
PhytoComm	Gua Lou	G241H1096523	61801	40	from supplier
PhytoComm	Gua Lou	G241H1096523	61878	40	from supplier
PhytoComm	Gua Lou	G241H1096621	61913	40	from supplier
PhytoComm	Gua Lou	G241H1096621	61914	40	from supplier
PhytoComm	Gua Lou	G241H1096821	62317	40	from supplier
PhytoComm	Gua Lou	G241H1096821	62318	40	from supplier
PhytoComm	Gua Lou	G241HS202SK1	62547	40	from supplier
PhytoComm	Gua Lou	G241HS202SK1	62548	40	from supplier

Validation samples

A total of 37 534 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 *Gua Lou*. These samples are listed above in the [calibration samples](#) section.
- 23 841 spectra from a total of 293 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 239 spectra of 10 reference samples from the substance/substance group *Gua Lou*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Gua Lou	G241H1096523	61787 [†]	20
PhytoComm	Gua Lou	G241H1096523	61801 [†]	20
PhytoComm	Gua Lou	G241H1096523	61877	59
PhytoComm	Gua Lou	G241H1096523	61878 [†]	20
PhytoComm	Gua Lou	G241H1096621	61913 [†]	20
PhytoComm	Gua Lou	G241H1096621	61914 [†]	20
PhytoComm	Gua Lou	G241H1096821	62317 [†]	20
PhytoComm	Gua Lou	G241H1096821	62318 [†]	20
PhytoComm	Gua Lou	G241HS202SK1	62547 [†]	20
PhytoComm	Gua Lou	G241HS202SK1	62548 [†]	20

- 12 243 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 3 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Gua Lou*.

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

Supplier	Substance	Batch	Spectra
Phytocomm	Gua Lou	G241H1096321	1
Phytocomm	Gua Lou	g241h1096321	1
Phytocomm	Gua Lou	G241H1096521	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	1	360	0	23 840
Type B	1	239	0	12 242
Type C	1	3	0	847

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	99.9924 % (> 99.9767 %)	100.0000 % (> 98.3333 %)
Type B	99.9848 % (> 99.9542 %)	100.0000 % (> 97.4895 %)
Type C	99.8457 % (> 99.2569 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61914	61914	0.00	11.02
62548	62548	0.00	4.49

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62318	62318	0.00	14.37
61913	61913	0.00	11.82
61801	61801	0.00	10.15
62547	62547	0.00	5.54
61787	61787	0.00	10.20
61878	61878	0.00	10.58
62317	62317	0.00	14.24

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Guang Huo Xiang**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 61079-2019-09-24
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	G007H2005822	62589	40	from supplier
PhytoComm	Guang Huo Xiang	G007H2005822	62590	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Guang Huo Xiang*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Guang Huo Xiang	G007H2005822	62589 [†]	20
PhytoComm	Guang Huo Xiang	G007H2005822	62590 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Guang Huo Xiang*.

Supplier	Substance	Batch	Spectra
Phytocomm	Guang Huo Xiang	G007H2005521	2

- 849 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	2	849

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62590	62590	0.00	24.41
62589	62589	0.00	24.57

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Gui Zhi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60189-2019-09-24
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	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

continued on the next page

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Gui Zhi	G070H1001624	62104	40	from supplier
PhytoComm	Gui Zhi	G070H1001821	62289	40	from supplier
PhytoComm	Gui Zhi	G070H1001821	62290	40	from supplier
PhytoComm	Gui Zhi	G070H1001822	62415	40	from supplier
PhytoComm	Gui Zhi	G070H1001822	62416	40	from supplier
PhytoComm	Gui Zhi	G070HS205SH1	62563	40	from supplier
PhytoComm	Gui Zhi	G070HS205SH1	62564	40	from supplier

Validation samples

A total of 37 534 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 560 spectra of 14 reference samples from the substance/substance group *Gui Zhi*. These samples are listed above in the [calibration samples](#) section.
- 23 641 spectra from a total of 292 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 280 spectra of 14 reference samples from the substance/substance group *Gui Zhi*.

Supplier	Substance	Batch	Sample ID	Spectra
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
PhytoComm	Gui Zhi	G070H1001821	62289 [†]	20
PhytoComm	Gui Zhi	G070H1001821	62290 [†]	20
PhytoComm	Gui Zhi	G070H1001822	62415 [†]	20
PhytoComm	Gui Zhi	G070H1001822	62416 [†]	20
PhytoComm	Gui Zhi	G070HS205SH1	62563 [†]	20
PhytoComm	Gui Zhi	G070HS205SH1	62564 [†]	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*.

- 12 202 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

Supplier	Substance	Batch	Spectra
Phytocomm	Gui Zhi	G070H1001221	2
Phytocomm	Gui Zhi	G070H1001422	1
Phytocomm	Gui Zhi	G070H100422	1
Phytocomm	Gui Zhi	G070H1001523	2

- 845 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	560	0	23 641
Type B	8	277	3	12 194
Type C	3	1	5	842

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 % (> 99.9686 %)	100.0000 % (> 98.9286 %)
Type B	99.9416 % (> 99.9110 %)	98.9286 % (> 97.8571 %)
Type C	99.3056 % (> 98.7157 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61873	61873	0.00	7.24
62415	62415	0.00	12.81
61815	61815	0.00	7.91
62065	62065	0.00	19.79
62564	62564	0.00	4.93
62103	62103	0.00	9.27
62066	62066	0.00	19.87
62289	62289	0.00	9.15
62563	62563	0.00	5.60
62290	62290	0.00	9.53
62104	62104	0.00	9.13
62416	62416	0.00	12.40
61777	61777	0.00	7.46
61874	61874	0.00	7.33

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Han Lian Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60540-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Han Lian Cao; Ecliptae prostratae herba

Special notes

When selecting the *Han Lian 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 *Han Lian Cao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Han Lian Cao	G095HS141RW1	62679	40	from supplier
PhytoComm	Han Lian Cao	G095HS141RW1	62680	40	from supplier

Validation samples

A total of 37 534 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 *Han Lian Cao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Han Lian Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Han Lian Cao	G095HS141RW1	62679 [†]	20
PhytoComm	Han Lian Cao	G095HS141RW1	62680 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 8 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Han Lian Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Han Lian Cao	G095H0770321	1
PhytoComm	Han Lian Cao	G095H0770321	2
Phytocomm	Han Lian Cao	g095h0770321	1
Phytocomm	Han Lian Cao	G095H0770521	4

- 843 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 sub-

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

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

Validation results

The validation runs checked whether the substance/substance group *Han Lian 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 *Han Lian 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	24 121
Type B	0	40	0	12 442
Type C	0	0	8	843

The substance/substance group *Han Lian 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8198 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62680	62680	0.00	9.45
62679	62679	0.00	6.23

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **He Huan Pi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60175-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

He Huan Pi; Albiziae 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	G010H0635822	62402	40	from supplier
PhytoComm	He Huan Pi	G010H0635822	62403	40	from supplier
PhytoComm	He Huan Pi	G010HS114SK1	62645	40	from supplier
PhytoComm	He Huan Pi	G010HS114SK1	62646	40	from supplier

Validation samples

A total of 37 534 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 *He Huan Pi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *He Huan Pi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	He Huan Pi	G010H0635822	62402 [†]	20
PhytoComm	He Huan Pi	G010H0635822	62403 [†]	20
PhytoComm	He Huan Pi	G010HS114SK1	62645 [†]	20
PhytoComm	He Huan Pi	G010HS114SK1	62646 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *He Huan Pi*.

Supplier	Substance	Batch	Spectra
Phytocomm	He Huan Pi	g010h0635221	1
Phytocomm	He Huan Pi	G010H0635423	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	8	157	3	24 033
Type B	12	77	3	12 390
Type C	0	1	1	849

The substance/substance group *He Huan 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	99.9441 % (> 99.9285 %)	98.1250 % (> 96.2500 %)
Type B	99.8285 % (> 99.7981 %)	96.2500 % (> 92.5000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62646	62646	0.00	3.45
62645	62645	0.00	3.72
62403	62403	0.00	15.55
62402	62402	0.00	15.27

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **He Shou Wu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60101-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

He Shou Wu; Polygoni multiflori radix

Special notes

When selecting the *He Shou Wu* substance/substance group, the following information is displayed to 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 Shou Wu*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	He Shou Wu	G198H0718821	62301	40	from supplier
PhytoComm	He Shou Wu	G198H0718821	62302	40	from supplier

Validation samples

A total of 37 534 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 Shou Wu*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	He Shou Wu	G198H0718821	62301 [†]	20
PhytoComm	He Shou Wu	G198H0718821	62302 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 7 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *He Shou Wu*.

Supplier	Substance	Batch	Spectra
Phytocomm	He Shou Wu	G198H0718222	1
Phytocomm	He Shou Wu	g198h0718222	1
PhytoComm	He Shou Wu	G198H0718222	1
Phytocomm	He Shou Wu	G198H0718421	3
PhytoComm	He Shou Wu	G198H0718421	1

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

- 844 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Shou Wu* 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 Shou Wu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 121
Type B	0	40	0	12 442
Type C	0	0	7	844

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8201 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62301	62301	0.00	12.23
62302	62302	0.00	12.74

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Hong Hua**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60206-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hong Hua; Carthami flos

Special notes

When selecting the *Hong 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 *Hong Hua*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Hong Hua	G057HS173SG1	62663	40	from supplier
PhytoComm	Hong Hua	G057HS173SG1	62664	40	from supplier

Validation samples

A total of 37 534 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 Hua*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Hong Hua*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Hong Hua	G057HS173SG1	62663 [†]	20
PhytoComm	Hong Hua	G057HS173SG1	62664 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Hong Hua*.

Supplier	Substance	Batch	Spectra
Phytocomm	Hong Hua	G057H0901221	1
Phytocomm	Hong Hua	g057h0901121	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 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 *Hong 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	24 121
Type B	0	40	0	12 442
Type C	0	0	2	849

The substance/substance group *Hong 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62663	62663	0.00	10.90
62664	62664	0.00	10.75

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Hong Jing Tian**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60031-2019-09-24
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
PhytoComm	Hong Jing Tian	G237H0906821	62305	40	from supplier
PhytoComm	Hong Jing Tian	G237H0906821	62306	40	from supplier
PhytoComm	Hong Jing Tian	G237HS429SK1	62639	40	from supplier
PhytoComm	Hong Jing Tian	G237HS429SK1	62640	40	from supplier

Validation samples

A total of 37 534 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 *Hong Jing Tian*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Hong Jing Tian*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Hong Jing Tian	G237H0906621	61911 [†]	20
PhytoComm	Hong Jing Tian	G237H0906621	61912 [†]	20
PhytoComm	Hong Jing Tian	G237H0906821	62305 [†]	20
PhytoComm	Hong Jing Tian	G237H0906821	62306 [†]	20
PhytoComm	Hong Jing Tian	G237HS429SK1	62639 [†]	20
PhytoComm	Hong Jing Tian	G237HS429SK1	62640 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Hong Jing Tian*.

Supplier	Substance	Batch	Spectra
Phytocomm	Hong Jing Tian	G237H0906321	1
Phytocomm	Hong Jing Tian	G237H0906221	1

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

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	118	2	12 362
Type C	0	0	2	849

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	98.3333 % (> 95.8333 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61912	61912	0.00	12.49
62639	62639	0.00	5.00
62305	62305	0.00	15.58
62640	62640	0.00	4.71
61911	61911	0.00	12.10
62306	62306	0.00	15.52

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Hou Po**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50289-2019-09-24
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	G154H0917822	62353	40	from supplier
PhytoComm	Hou Po	G154H0917822	62354	40	from supplier
PhytoComm	Hou Po	G154HS184SH1	62613	40	from supplier
PhytoComm	Hou Po	G154HS184SH1	62614	40	from supplier

Validation samples

A total of 37 534 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 *Hou Po*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Hou Po*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Hou Po	G154H0917822	62353 [†]	20
PhytoComm	Hou Po	G154H0917822	62354 [†]	20
PhytoComm	Hou Po	G154HS184SH1	62613 [†]	20
PhytoComm	Hou Po	G154HS184SH1	62614 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Hou Po*.

Supplier	Substance	Batch	Spectra
Phytocomm	Hou Po	G154H0917222	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	1	160	0	24 040
Type B	0	80	0	12 402
Type C	1	0	1	849

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	99.9924 % (> 99.9767 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.8843 % (> 99.2998 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62353	62353	0.00	13.86
62614	62614	0.00	7.15
62354	62354	0.00	13.99
62613	62613	0.00	7.09

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Hu Zhang**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60130-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hu Zhang; Polygoni cuspidati rhizoma et radix

Special notes

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Hu Zhang	G197HS373SK1	62565	40	from supplier
PhytoComm	Hu Zhang	G197HS373SK1	62566	40	from supplier

Validation samples

A total of 37 534 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 *Hu Zhang*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Hu Zhang	G197HS373SK1	62565 [†]	20
PhytoComm	Hu Zhang	G197HS373SK1	62566 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Hu Zhang*.

Supplier	Substance	Batch	Spectra
Phytocomm	Hu Zhang	G197H0851321	1
Phytocomm	Hu Zhang	g197h0851321	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

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

Validation results

The validation runs checked whether the substance/substance group *Hu Zhang* 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 *Hu Zhang* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 121
Type B	0	40	0	12 442
Type C	0	0	2	849

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62565	62565	0.00	13.07
62566	62566	0.00	13.28

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Hua Shi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50308-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hua Shi; Talcum

Special notes

When selecting the *Hua Shi* substance/substance group, the following information is displayed to 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 *Hua Shi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Hua Shi	G238HS289RM1	62425	40	from supplier
PhytoComm	Hua Shi	G238HS289RM1	62426	40	from supplier
PhytoComm	Hua Shi	G238HS289SK1	62637	40	from supplier
PhytoComm	Hua Shi	G238HS289SK1	62638	40	from supplier

Validation samples

A total of 37 534 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 *Hua Shi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Hua Shi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Hua Shi	G238HS289RM1	62425 [†]	20
PhytoComm	Hua Shi	G238HS289RM1	62426 [†]	20
PhytoComm	Hua Shi	G238HS289SK1	62637 [†]	20
PhytoComm	Hua Shi	G238HS289SK1	62638 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Hua Shi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Hua Shi	g238h1332121	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

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

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	68	92	24 041
Type B	0	29	51	12 402
Type C	0	0	1	850

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9687 %)	42.5000 % (> 40.6250 %)
Type B	100.0000 % (> 99.9391 %)	36.2500 % (> 32.5000 %)
Type C	100.0000 % (> 98.8311 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62426	62426	0.00	569.59
62638	62638	0.00	615.19
62637	62637	0.00	612.72
62425	62425	0.00	551.43

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Huang Bo**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60057-2019-09-24
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	G188H1203823	62593	40	from supplier
PhytoComm	Huang Bo	G188H1203823	62594	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Huang Bo*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huang Bo	G188H1203823	62593 [†]	20
PhytoComm	Huang Bo	G188H1203823	62594 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 6 spectra from 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Huang Bo*.

Supplier	Substance	Batch	Spectra
Phytocomm	Huang Bo	g188h1203123	1
Phytocomm	Huang Bo	h1203022	1
PhytoComm	Huang Bo	G188H1203321	1
Phytocomm	Huang Bo	G188H1203321	3

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	1	2	4	844

The substance/substance group *Huang Bo* 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.9339 % (> 99.3440 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62593	62593	0.00	19.09
62594	62594	0.00	19.24

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Huang Jing**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60108-2019-09-24
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	G196H1206721	62303	40	from supplier
PhytoComm	Huang Jing	G196H1206721	62304	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Huang Jing*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huang Jing	G196H1206721	62303 [†]	20
PhytoComm	Huang Jing	G196H1206721	62304 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Huang Jing*.

Supplier	Substance	Batch	Spectra
Phytocomm	Huang Jing	g196h1206121	1
Phytocomm	Huang Jing	G196H1206121	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	2	849

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62304	62304	0.00	13.36
62303	62303	0.00	12.66

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Huang Lian**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60219-2019-09-24
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	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
PhytoComm	Huang Lian	G079HS261RM1	62287	40	from supplier
PhytoComm	Huang Lian	G079HS261RM1	62288	40	from supplier

Validation samples

A total of 37 534 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 *Huang Lian*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Huang Lian*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huang Lian	G079H1205621	61776 [†]	20
PhytoComm	Huang Lian	G079H1205621	61819 [†]	20
PhytoComm	Huang Lian	G079H1205622	62091 [†]	20
PhytoComm	Huang Lian	G079H1205622	62092 [†]	20
PhytoComm	Huang Lian	G079HS261RM1	62287 [†]	20
PhytoComm	Huang Lian	G079HS261RM1	62288 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 12 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Huang Lian*.

Supplier	Substance	Batch	Spectra
Phytocomm	Huang Lian	G079H1205321	2

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

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Supplier	Substance	Batch	Spectra
PhytoComm	Huang Lian	G079H1205321	4
Phytocomm	Huang Lian	g079h1205321	1
Phytocomm	Huang Lian	G079H1205521	2
Phytocomm	Huang Lian	G079H1205421	1
PhytoComm	Huang Lian	G079H1205521	2

- 839 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	12	0	839

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8193 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62092	62092	0.00	25.75
62091	62091	0.00	25.70
62287	62287	0.00	13.71
62288	62288	0.00	14.02
61819	61819	0.00	24.72
61776	61776	0.00	25.38

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Huang Qi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60154-2019-09-24
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
PhytoComm	Huang Qi	G040H1202822	62383	40	from supplier
PhytoComm	Huang Qi	G040H1202822	62384	40	from supplier
PhytoComm	Huang Qi	G040H1202823	62511	40	from supplier
PhytoComm	Huang Qi	G040H1202823	62512	40	from supplier

Validation samples

A total of 37 534 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 *Huang Qi*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Huang Qi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huang Qi	G040H1202721	62227 [†]	20
PhytoComm	Huang Qi	G040H1202721	62228 [†]	20
PhytoComm	Huang Qi	G040H1202822	62383 [†]	20
PhytoComm	Huang Qi	G040H1202822	62384 [†]	20
PhytoComm	Huang Qi	G040H1202823	62511 [†]	20
PhytoComm	Huang Qi	G040H1202823	62512 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 10 spectra from 5 *Apo-Ident* customers from 6 batches from the substance/substance group *Huang Qi*.

Supplier	Substance	Batch	Spectra
PhytoComm	Huang Qi	G040H1202321	1

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

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Supplier	Substance	Batch	Spectra
Phytocomm	Huang Qi	G040H1202321	1
Phytocomm	Huang Qi	g040h1202321	2
Phytocomm	Huang Qi	G040H1202423	2
Caelo	Huang Qi	g040h1202222	1
Phytocomm	Huang Qi	G040H1202521	2
PhytoComm	Huang Qi	G040H1202621	1

- 841 spectra from 12 *Apo-Ident* customers from a total of 507 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	1	120	0	12 361
Type C	1	2	8	840

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	99.9848 % (> 99.9543 %)	100.0000 % (> 95.0000 %)
Type C	99.7685 % (> 99.1783 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62512	62512	0.00	11.26
62228	62228	0.00	9.91
62383	62383	0.00	15.04
62227	62227	0.00	11.20
62511	62511	0.00	11.19
62384	62384	0.00	14.47

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Huang Qin**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60012-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Huang Qin; Scutellariae baicalensis radix

Special notes

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Huang Qin	G225HS259RM1	62281	40	from supplier
PhytoComm	Huang Qin	G225HS259RM1	62282	40	from supplier

Validation samples

A total of 37 534 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 Qin*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Huang Qin*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huang Qin	G225HS259RM1	62281 [†]	20
PhytoComm	Huang Qin	G225HS259RM1	62282 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 12 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Huang Qin*.

Supplier	Substance	Batch	Spectra
Phytocomm	Huang Qin	G225H1204221	1
PhytoComm	Huang Qin	G225H1204221	1
Phytocomm	Huang Qin	g225h1204121	1
PhytoComm	Huang Qin	G225H1204322	5
Herbasin	Huang Qin	g225h120442	1
Phytocomm	Huang Qin	G225H1204522	3

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

- 839 spectra from 12 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Qin* 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 Qin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 121
Type B	0	40	0	12 442
Type C	0	0	12	839

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8193 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62282	62282	0.00	20.87
62281	62281	0.00	21.59

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Huo Ma Ren**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60234-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Huo Ma Ren; Lini semen

Special notes

When selecting the *Huo Ma 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 *Huo Ma Ren*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Huo Ma Ren	G141H0449823	62411	40	from supplier
PhytoComm	Huo Ma Ren	G141H0449823	62412	40	from supplier

Validation samples

A total of 37 534 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 *Huo Ma Ren*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Huo Ma Ren*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Huo Ma Ren	G141H0449823	62411 [†]	20
PhytoComm	Huo Ma Ren	G141H0449823	62412 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Huo Ma Ren*.

Supplier	Substance	Batch	Spectra
Phytocomm	Huo Ma Ren	G141HS061	2

- 849 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

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

Validation results

The validation runs checked whether the substance/substance group *Huo Ma 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 *Huo Ma 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	24 121
Type B	0	40	0	12 442
Type C	0	0	2	849

The substance/substance group *Huo Ma 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62412	62412	0.00	11.21
62411	62411	0.00	11.62

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ji Li**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60110-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ji Li; Tribuli terrestris fructus

Special notes

When selecting the *Ji Li* substance/substance group, the following information is displayed to 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 *Ji Li*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ji Li	G240H1410821	62319	40	from supplier
PhytoComm	Ji Li	G240H1410821	62320	40	from supplier
PhytoComm	Ji Li	G240HS305SK1	62545	40	from supplier
PhytoComm	Ji Li	G240HS305SK1	62546	40	from supplier

Validation samples

A total of 37 534 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 *Ji Li*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ji Li	G240H1410821	62319 [†]	20
PhytoComm	Ji Li	G240H1410821	62320 [†]	20
PhytoComm	Ji Li	G240HS305SK1	62545 [†]	20
PhytoComm	Ji Li	G240HS305SK1	62546 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Ji Li*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ji Li	G240H1410421	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

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

Validation results

The validation runs checked whether the substance/substance group *Ji Li* 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 *Ji Li* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 041
Type B	3	80	0	12 399
Type C	1	0	1	849

The substance/substance group *Ji Li* 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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	99.9771 % (> 99.9467 %)	100.0000 % (> 92.5000 %)
Type C	99.9228 % (> 99.3384 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62319	62319	0.00	10.66
62546	62546	0.00	6.14
62545	62545	0.00	5.56
62320	62320	0.00	10.35

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ji Xue Teng**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60099-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ji Xue Teng; Spatholobi caulis

Special notes

When selecting the *Ji Xue 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 *Ji Xue Teng*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ji Xue Teng	G159HS337SK1	62559	40	from supplier
PhytoComm	Ji Xue Teng	G159HS337SK1	62560	40	from supplier

Validation samples

A total of 37 534 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 *Ji Xue Teng*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Ji Xue Teng*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ji Xue Teng	G159HS337SK1	62559 [†]	20
PhytoComm	Ji Xue Teng	G159HS337SK1	62560 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Ji Xue Teng*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ji Xue Teng	G159H2101423	3
Phytocomm	Ji Xue Teng	g159h2101122	1

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

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

Validation results

The validation runs checked whether the substance/substance group *Ji Xue 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 *Ji Xue 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	5	77	3	24 116
Type B	5	40	0	12 437
Type C	0	0	4	847

The substance/substance group *Ji Xue Teng* 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	99.9873 % (> 99.9717 %)	96.2500 % (> 92.5000 %)
Type B	99.9746 % (> 99.9443 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62559	62559	0.00	4.48
62560	62560	0.00	4.43

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Jiang Huang**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60181-2019-09-24
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	G085H1716721	62373	40	from supplier
PhytoComm	Jiang Huang	G085H1716721	62374	40	from supplier
PhytoComm	Jiang Huang	G085H1716821	62519	40	from supplier
PhytoComm	Jiang Huang	G085H1716821	62520	40	from supplier

Validation samples

A total of 37 534 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 *Jiang Huang*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jiang Huang	G085H1716721	62373 [†]	20
PhytoComm	Jiang Huang	G085H1716721	62374 [†]	20
PhytoComm	Jiang Huang	G085H1716821	62519 [†]	20
PhytoComm	Jiang Huang	G085H1716821	62520 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

Supplier	Substance	Batch	Spectra
Phytocomm	Jiang Huang	G085H1716422	3
PhytoComm	Jiang Huang	G085H1716321	1
PhytoComm	Jiang Huang	G085H1716422	1

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

- 846 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	2	2	3	844

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.5370 % (> 98.9474 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62520	62520	0.00	7.61
62373	62373	0.00	15.53
62374	62374	0.00	15.79
62519	62519	0.00	7.82

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Jiao Gu Lan**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60332-2019-09-24
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	G065HS424RR1	62441	40	from supplier
PhytoComm	Jiao Gu Lan	G065HS424RR1	62442	40	from supplier
PhytoComm	Jiao Gu Lan	G065HS424SG1	62665	40	from supplier
PhytoComm	Jiao Gu Lan	G065HS424SG1	62666	40	from supplier

Validation samples

A total of 37 534 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 *Jiao Gu Lan*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Jiao Gu Lan*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jiao Gu Lan	G065HS424RR1	62441 [†]	20
PhytoComm	Jiao Gu Lan	G065HS424RR1	62442 [†]	20
PhytoComm	Jiao Gu Lan	G065HS424SG1	62665 [†]	20
PhytoComm	Jiao Gu Lan	G065HS424SG1	62666 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 3 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Jiao Gu Lan*.

Supplier	Substance	Batch	Spectra
Phytocomm	Jiao Gu Lan	G065FB1276421	3

- 848 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	3	848

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62666	62666	0.00	10.83
62441	62441	0.00	8.32
62665	62665	0.00	10.62
62442	62442	0.00	9.97

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Jie Geng**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60034-2019-09-24
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
PhytoComm	Jie Geng	G193H1015821	62365	40	from supplier
PhytoComm	Jie Geng	G193H1015821	62366	40	from supplier

Validation samples

A total of 37 534 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 *Jie Geng*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Jie Geng*.

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
PhytoComm	Jie Geng	G193H1015821	62365 [†]	20
PhytoComm	Jie Geng	G193H1015821	62366 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

Supplier	Substance	Batch	Spectra
Phytocomm	Jie Geng	g193h1015221	1
Phytocomm	Jie Geng	G193H1015521	4

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

- 846 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	1	236	4	23 960
Type B	4	113	7	12 358
Type C	4	4	1	842

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	99.9978 % (> 99.9822 %)	98.3333 % (> 97.0833 %)
Type B	99.9826 % (> 99.9521 %)	94.1667 % (> 91.6667 %)
Type C	99.6399 % (> 99.0503 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well 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	9.12
61932	61932	0.00	8.64
62247	62247	0.00	3.63
62365	62365	0.00	8.34
62366	62366	0.00	8.07
62248	62248	0.00	4.25

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Jin Qian Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50293-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Jin Qian Cao; Lysimachiae herba

Special notes

When selecting the *Jin Qian 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 *Jin Qian Cao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Jin Qian Cao	G151H0847821	62465	40	from supplier
PhytoComm	Jin Qian Cao	G151H0847821	62466	40	from supplier

Validation samples

A total of 37 534 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 Qian Cao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Jin Qian Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jin Qian Cao	G151H0847821	62465 [†]	20
PhytoComm	Jin Qian Cao	G151H0847821	62466 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Jin Qian Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Jin Qian Cao	g151h0847122	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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 Qian 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 *Jin Qian 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	24 121
Type B	0	40	0	12 442
Type C	0	0	1	850

The substance/substance group *Jin Qian 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8311 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62465	62465	0.00	18.73
62466	62466	0.00	18.78

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Jin Yin Hua**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60350-2019-09-24
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
PhytoComm	Jin Yin Hua	G145HS311SK1	62577	40	from supplier
PhytoComm	Jin Yin Hua	G145HS311SK1	62578	40	from supplier

Validation samples

A total of 37 534 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 *Jin Yin Hua*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Jin Yin Hua*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jin Yin Hua	G145HS311QG1	62189 [†]	20
PhytoComm	Jin Yin Hua	G145HS311QG1	62190 [†]	20
PhytoComm	Jin Yin Hua	G145HS311SK1	62577 [†]	20
PhytoComm	Jin Yin Hua	G145HS311SK1	62578 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Jin Yin Hua*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

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

Validation results

The validation runs checked whether the substance/substance group *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	160	0	24 041
Type B	2	80	0	12 400
Type C	1	0	0	850

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	99.9898 % (> 99.9594 %)	100.0000 % (> 92.5000 %)
Type C	99.7685 % (> 99.1776 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well 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	9.27
62578	62578	0.00	8.68
62190	62190	0.00	10.28
62577	62577	0.00	8.88

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Jing Jie**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60088-2019-09-24
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	G221H1038822	62497	40	from supplier
PhytoComm	Jing Jie	G221H1038822	62498	40	from supplier

Validation samples

A total of 37 534 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 *Jing Jie*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Jing Jie*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Jing Jie	G221H1038822	62497 [†]	20
PhytoComm	Jing Jie	G221H1038822	62498 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Jing Jie*.

Supplier	Substance	Batch	Spectra
Phytocomm	Jing Jie	G221H1038221	1
Phytocomm	Jing Jie	g221h1038221	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	40	0	12 442
Type C	0	0	2	849

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62498	62498	0.00	8.91
62497	62497	0.00	8.56

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ju Hua**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60232-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Ju Hua*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ju Hua	G064H1231521	62023 [†]	20
PhytoComm	Ju Hua	G064H1231521	62024 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Ju Hua*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ju Hua	G064H1231421	2
PhytoComm	Ju Hua	G064H1231421	1
PhytoComm	Ju Hua	G064H1231521	1

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	1	4	0	846

The substance/substance group *Ju 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.7685 % (> 99.1792 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62024	62024	0.00	14.24
62023	62023	0.00	14.43

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ku Shen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60112-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ku Shen; Sophorae flavescens 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
PhytoComm	Ku Shen	G233H0908822	62499	40	from supplier
PhytoComm	Ku Shen	G233H0908822	62500	40	from supplier

Validation samples

A total of 37 534 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 *Ku Shen*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Ku Shen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ku Shen	G233H0908521	61927 [†]	20
PhytoComm	Ku Shen	G233H0908521	61928 [†]	20
PhytoComm	Ku Shen	G233H0908822	62499 [†]	20
PhytoComm	Ku Shen	G233H0908822	62500 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Ku Shen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ku Shen	G233H0908121	1
Phytocomm	Ku Shen	h0908121	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	1	0	2	848

The substance/substance group *Ku 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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.8457 % (> 99.2580 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62500	62500	0.00	13.72
62499	62499	0.00	14.00
61928	61928	0.00	21.09
61927	61927	0.00	21.53

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Lai Fu Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60067-2019-09-24
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	G209H1220821	62491	40	from supplier
PhytoComm	Lai Fu Zi	G209H1220821	62492	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Lai Fu Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Lai Fu Zi	G209H1220821	62491 [†]	20
PhytoComm	Lai Fu Zi	G209H1220821	62492 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 3 spectra from 1 *Apo-Ident* customers from 3 batches from the substance/substance group *Lai Fu Zi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Lai Fu Zi	G209H1220221	1
Phytocomm	Lai Fu Zi	G209H1220321	1
Herbasin	Lai Fu Zi	g209h1220321	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	3	848

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62491	62491	0.00	12.32
62492	62492	0.00	11.52

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Lian Qiao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60146-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lian Qiao; Forsythiae 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
PhytoComm	Lian Qiao	G105H1132821	62337	40	from supplier
PhytoComm	Lian Qiao	G105H1132821	62338	40	from supplier
PhytoComm	Lian Qiao	G105HS252RW1	62685	40	from supplier
PhytoComm	Lian Qiao	G105HS252RW1	62686	40	from supplier

Validation samples

A total of 37 534 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 *Lian Qiao*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Lian Qiao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Lian Qiao	G105H1132721	62231 [†]	20
PhytoComm	Lian Qiao	G105H1132721	62232 [†]	20
PhytoComm	Lian Qiao	G105H1132821	62337 [†]	20
PhytoComm	Lian Qiao	G105H1132821	62338 [†]	20
PhytoComm	Lian Qiao	G105HS252RW1	62685 [†]	20
PhytoComm	Lian Qiao	G105HS252RW1	62686 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 3 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Lian Qiao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Lian Qiao	G105H1132221	1
PhytoComm	Lian Qiao	G105H1132321	1
Phytocomm	Lian Qiao	G105H1132521	1

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

- 848 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	239	1	23 961
Type B	2	119	1	12 360
Type C	1	0	3	847

The substance/substance group *Lian Qiao* 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 % (> 99.9687 %)	99.5833 % (> 98.3333 %)
Type B	99.9898 % (> 99.9594 %)	99.1667 % (> 96.6667 %)
Type C	99.8843 % (> 99.2955 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62686	62686	0.00	4.95
62338	62338	0.00	17.09
62231	62231	0.00	10.21
62337	62337	0.00	17.22
62685	62685	0.00	5.41
62232	62232	0.00	11.16

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Lian Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60248-2019-09-24
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	40	from supplier
PhytoComm	Lian Zi	G171HS312SK1	62567	40	from supplier
PhytoComm	Lian Zi	G171HS312SK1	62568	40	from supplier

Validation samples

A total of 37 534 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 *Lian Zi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Lian Zi	G171HS312QM1	62197 [†]	20
PhytoComm	Lian Zi	G171HS312QM1	62198 [†]	20
PhytoComm	Lian Zi	G171HS312SK1	62567 [†]	20
PhytoComm	Lian Zi	G171HS312SK1	62568 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Lian Zi*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

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

Validation results

The validation runs checked whether the substance/substance group *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	0	160	0	24 041
Type B	3	78	2	12 399
Type C	0	0	0	851

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	100.0000 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	99.9848 % (> 99.9543 %)	97.5000 % (> 93.7500 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62568	62568	0.00	4.71
62198	62198	0.00	6.67
62567	62567	0.00	5.09
62197	62197	0.00	6.72

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ling Zhi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60187-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ling Zhi; Ganoderma

Special notes

When selecting the *Ling 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 *Ling Zhi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ling Zhi	G109HS355RP1	62453	40	from supplier
PhytoComm	Ling Zhi	G109HS355RP1	62454	40	from supplier

Validation samples

A total of 37 534 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 *Ling Zhi*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ling Zhi	G109HS355RP1	62453 [†]	20
PhytoComm	Ling Zhi	G109HS355RP1	62454 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Ling Zhi*.

Supplier	Substance	Batch	Spectra
PhytoComm	Ling Zhi	G109F-B2405221	1
Phytocomm	Ling Zhi	g109fb2405321	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

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

Validation results

The validation runs checked whether the substance/substance group *Ling 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 *Ling 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	79	1	24 121
Type B	2	40	0	12 440
Type C	0	0	2	849

The substance/substance group *Ling 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 % (> 99.9689 %)	98.7500 % (> 95.0000 %)
Type B	99.9848 % (> 99.9545 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62454	62454	0.00	6.42
62453	62453	0.00	5.75

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Long Dan (Cao)**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60227-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Long Dan (Cao); 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
PhytoComm	Long Dan (Cao)	G112H1705821	62531	40	from supplier
PhytoComm	Long Dan (Cao)	G112H1705821	62532	40	from supplier

Validation samples

A total of 37 534 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 161 spectra of 4 reference samples from the substance/substance group *Long Dan (Cao)*. These samples are listed above in the [calibration samples](#) section.
- 24 040 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Long Dan (Cao)*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Long Dan (Cao)	G112H1705621	62123 [†]	20
PhytoComm	Long Dan (Cao)	G112H1705621	62124 [†]	20
PhytoComm	Long Dan (Cao)	G112H1705821	62531 [†]	20
PhytoComm	Long Dan (Cao)	G112H1705821	62532 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Long Dan (Cao)*.

Supplier	Substance	Batch	Spectra
Phytocomm	Long Dan (Cao)	g112h1705022	1
Phytocomm	Long Dan (Cao)	G112H1705321	3

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

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

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	161	0	24 040
Type B	0	80	0	12 402
Type C	0	0	4	847

The substance/substance group *Long Dan (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 % (> 99.9687 %)	100.0000 % (> 96.2733 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62532	62532	0.00	13.09
62123	62123	0.00	9.92
62124	62124	0.00	10.55
62531	62531	0.00	13.62

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Long Yan Rou**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60463-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Long Yan Rou; Euphoriae longanae 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
PhytoComm	Long Yan Rou	G144HS324RN1	62267	40	from supplier
PhytoComm	Long Yan Rou	G144HS324RN1	62268	40	from supplier

Validation samples

A total of 37 534 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 *Long Yan Rou*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 4 reference samples from the substance/substance group *Long Yan Rou*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Long Yan Rou	G144HS324PW1	62203 [†]	20
PhytoComm	Long Yan Rou	G144HS324PW1	62204 [†]	20
PhytoComm	Long Yan Rou	G144HS324RN1	62267 [†]	20
PhytoComm	Long Yan Rou	G144HS324RN1	62268 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Long Yan Rou*.

Supplier	Substance	Batch	Spectra
PhytoComm	Long Yan Rou	G144H1708221	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	1	850

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8311 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62204	62204	0.00	5.69
62268	62268	0.00	13.02
62203	62203	0.00	5.53
62267	62267	0.00	13.85

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Lu Gen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60259-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lu Gen; Phragmitis communis rhizoma

Special notes

When selecting the *Lu 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 *Lu Gen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Lu Gen	G189H2014821	62485	40	from supplier
PhytoComm	Lu Gen	G189H2014821	62486	40	from supplier

Validation samples

A total of 37 534 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 Gen*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Lu Gen	G189H2014821	62485 [†]	20
PhytoComm	Lu Gen	G189H2014821	62486 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Lu Gen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Lu Gen	G189H2014221	1
Phytocomm	Lu Gen	G189H2014521	1
PhytoComm	Lu Gen	G189H2014521	2

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

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

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 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 *Lu 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	24 121
Type B	0	40	0	12 442
Type C	1	0	4	846

The substance/substance group *Lu 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.8843 % (> 99.2950 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62486	62486	0.00	7.13
62485	62485	0.00	7.41

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ma Bian Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60479-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ma Bian Cao; Verbenae officinalis herba

Special notes

When selecting the *Ma Bian 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 *Ma Bian Cao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Ma Bian Cao	G248H1085823	62591	40	from supplier
PhytoComm	Ma Bian Cao	G248H1085823	62592	40	from supplier

Validation samples

A total of 37 534 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 *Ma Bian Cao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Ma Bian Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ma Bian Cao	G248H1085823	62591 [†]	20
PhytoComm	Ma Bian Cao	G248H1085823	62592 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Ma Bian Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ma Bian Cao	G248H1085221	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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 Bian 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 *Ma Bian 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	2	80	0	24 119
Type B	2	39	1	12 440
Type C	1	0	1	849

The substance/substance group *Ma Bian 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	99.9924 % (> 99.9768 %)	100.0000 % (> 92.5000 %)
Type B	99.9848 % (> 99.9545 %)	97.5000 % (> 90.0000 %)
Type C	99.9228 % (> 99.3384 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62592	62592	0.00	5.01
62591	62591	0.00	4.74

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ma Huang**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50283-2019-09-24
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	G097H1101623	62147	40	from supplier
PhytoComm	Ma Huang	G097H1101623	62148	40	from supplier
PhytoComm	Ma Huang	G097HS255RT1	62681	40	from supplier
PhytoComm	Ma Huang	G097HS255RT1	62682	40	from supplier
PhytoComm	Ma Huang	G097HS255SL1	62693	40	from supplier
PhytoComm	Ma Huang	G097HS255SL1	62694	40	from supplier

Validation samples

A total of 37 534 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 *Ma Huang*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Ma Huang*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ma Huang	G097H1101623	62147 [†]	20
PhytoComm	Ma Huang	G097H1101623	62148 [†]	20
PhytoComm	Ma Huang	G097HS255RT1	62681 [†]	20
PhytoComm	Ma Huang	G097HS255RT1	62682 [†]	20
PhytoComm	Ma Huang	G097HS255SL1	62693 [†]	20
PhytoComm	Ma Huang	G097HS255SL1	62694 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Ma Huang*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ma Huang	G097H1101522	2

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

- 849 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	0	2	849

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62694	62694	0.00	7.43
62693	62693	0.00	8.22
62148	62148	0.00	42.27
62682	62682	0.00	13.55
62147	62147	0.00	42.53
62681	62681	0.00	13.64

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ma Huang Gen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60063-2019-09-24
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	G278HS393RN1	62261	40	from supplier
PhytoComm	Ma Huang Gen	G278HS393RN1	62262	40	from supplier

Validation samples

A total of 37 534 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 *Ma Huang Gen*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 40 spectra of 2 reference samples from the substance/substance group *Ma Huang Gen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ma Huang Gen	G278HS393RN1	62261 [†]	20
PhytoComm	Ma Huang Gen	G278HS393RN1	62262 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ma Huang Gen*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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

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

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	1	79	1	24 120
Type B	3	37	3	12 439
Type C	1	0	0	850

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	99.9975 % (> 99.9819 %)	98.7500 % (> 95.0000 %)
Type B	99.9848 % (> 99.9545 %)	92.5000 % (> 85.0000 %)
Type C	99.8843 % (> 99.2934 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62261	62261	0.00	3.15
62262	62262	0.00	5.99

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Mai Men Dong**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60024-2019-09-24
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
PhytoComm	Mai Men Dong	G176HS236SH1	62611	40	from supplier
PhytoComm	Mai Men Dong	G176HS236SH1	62612	40	from supplier

Validation samples

A total of 37 534 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 *Mai Men Dong*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 6 reference samples from the substance/substance group *Mai Men Dong*.

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
PhytoComm	Mai Men Dong	G176HS236SH1	62611 [†]	20
PhytoComm	Mai Men Dong	G176HS236SH1	62612 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 4 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Mai Men Dong*.

Supplier	Substance	Batch	Spectra
Phytocomm	Mai Men Dong	g176h1118221	1
Phytocomm	Mai Men Dong	G176H1118521	3

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

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	3	1	847

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62611	62611	0.00	12.61
62114	62114	0.00	12.93
62612	62612	0.00	11.62
61945	61945	0.00	16.61
61946	61946	0.00	16.84
62113	62113	0.00	12.30

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Mai Ya**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60210-2019-09-24
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	G123H1119821	62535	40	from supplier
PhytoComm	Mai Ya	G123H1119821	62536	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Mai Ya*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mai Ya	G123H1119821	62535 [†]	20
PhytoComm	Mai Ya	G123H1119821	62536 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Mai Ya*.

Supplier	Substance	Batch	Spectra
Phytocomm	Mai Ya	g123h1119022	1
Phytocomm	Mai Ya	G123H1119521	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	2	849

The substance/substance group *Mai Ya* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62536	62536	0.00	9.35
62535	62535	0.00	9.46

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Man Jing Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60025-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Man Jing Zi; Vitis 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	G250H1505822	62501	40	from supplier
PhytoComm	Man Jing Zi	G250H1505822	62502	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Man Jing Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Man Jing Zi	G250H1505822	62501 [†]	20
PhytoComm	Man Jing Zi	G250H1505822	62502 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Man Jing Zi*.

Supplier	Substance	Batch	Spectra
PhytoComm	Man Jing Zi	G250H1505122	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	1	850

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8311 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62501	62501	0.00	30.79
62502	62502	0.00	30.74

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Mang Xiao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50387-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Mang Xiao; Mirabilitum

Special notes

When selecting the *Mang Xiao* substance/substance group, the following information is displayed to 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 *Mang Xiao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Mang Xiao	G160H0627821	62469	40	from supplier
PhytoComm	Mang Xiao	G160H0627821	62470	40	from supplier

Validation samples

A total of 37 534 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 *Mang Xiao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 160 spectra of 4 reference samples from the substance/substance group *Mang Xiao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mang Xiao	G160H0627623	62241	60
PhytoComm	Mang Xiao	G160H0627623	62242	60
PhytoComm	Mang Xiao	G160H0627821	62469 [†]	20
PhytoComm	Mang Xiao	G160H0627821	62470 [†]	20

- 12 322 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Mang Xiao*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Mang Xiao* 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 *Mang Xiao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 121
Type B	0	160	0	12 322
Type C	0	0	0	851

The substance/substance group *Mang Xiao* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9390 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62470	62470	0.00	46.00
62469	62469	0.00	45.72

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Mao Dong Qing**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60028-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Mao Dong Qing; Ilicis pubescendis radix

Special notes

When selecting the *Mao Dong Qing* substance/substance group, the following information is displayed to 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 *Mao Dong Qing*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Mao Dong Qing	G319HS063RN1	62417	40	from supplier
PhytoComm	Mao Dong Qing	G319HS063RN1	62418	40	from supplier
PhytoComm	Mao Dong Qing	G319HS063SK1	62619	40	from supplier
PhytoComm	Mao Dong Qing	G319HS063SK1	62620	40	from supplier

Validation samples

A total of 37 534 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 *Mao Dong Qing*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Mao Dong Qing*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mao Dong Qing	G319HS063RN1	62417 [†]	20
PhytoComm	Mao Dong Qing	G319HS063RN1	62418 [†]	20
PhytoComm	Mao Dong Qing	G319HS063SK1	62619 [†]	20
PhytoComm	Mao Dong Qing	G319HS063SK1	62620 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Mao Dong Qing*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Mao Dong Qing* 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 *Mao Dong Qing* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 041
Type B	3	80	0	12 399
Type C	0	0	0	851

The substance/substance group *Mao Dong Qing* 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 % (> 99.9687 %)	99.3750 % (> 97.5000 %)
Type B	99.9797 % (> 99.9492 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62620	62620	0.00	9.46
62418	62418	0.00	6.82
62619	62619	0.00	9.40
62417	62417	0.00	7.41

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Mo Yao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50343-2019-09-24
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	G169H0732823	62479	40	from supplier
PhytoComm	Mo Yao	G169H0732823	62480	40	from supplier

Validation samples

A total of 37 534 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 *Mo Yao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Mo Yao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mo Yao	G169H0732823	62479 [†]	20
PhytoComm	Mo Yao	G169H0732823	62480 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Mo Yao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Mo Yao	G1690732222	1
Caelo	Mo Yao	G169H0732222	1
PhytoComm	Mo Yao	G169H0732222	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	40	0	12 442
Type C	0	0	3	848

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62480	62480	0.00	13.24
62479	62479	0.00	13.62

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Mu Dan Pi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60113-2019-09-24
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	G166HS129RT1	62433	40	from supplier
PhytoComm	Mu Dan Pi	G166HS129RT1	62434	40	from supplier
PhytoComm	Mu Dan Pi	G166H0741821	62475	40	from supplier
PhytoComm	Mu Dan Pi	G166H0741821	62476	40	from supplier

Validation samples

A total of 37 534 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 *Mu Dan Pi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Mu Dan Pi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mu Dan Pi	G166HS129RT1	62433 [†]	20
PhytoComm	Mu Dan Pi	G166HS129RT1	62434 [†]	20
PhytoComm	Mu Dan Pi	G166H0741821	62475 [†]	20
PhytoComm	Mu Dan Pi	G166H0741821	62476 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 11 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Mu Dan Pi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Mu Dan Pi	G166H0741122	2
Phytocomm	Mu Dan Pi	G166H0741121	1
Phytocomm	Mu Dan Pi	G166H0741321	2
Phytocomm	Mu Dan Pi	g166j074122	1
PhytoComm	Mu Dan Pi	G166H0741321	1
Phytocomm	Mu Dan Pi	G166H0741421	4

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 840 spectra from 12 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	77	3	12 402
Type C	0	0	11	840

The substance/substance group *Mu Dan 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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	96.2500 % (> 92.5000 %)
Type C	100.0000 % (> 98.8194 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62475	62475	0.00	10.64
62434	62434	0.00	5.34
62433	62433	0.00	5.56
62476	62476	0.00	10.43

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Mu Gua**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60236-2019-09-24
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	G063H0424621	62085	40	from supplier
PhytoComm	Mu Gua	G063H0424621	62086	40	from supplier

Validation samples

A total of 37 534 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 Gua*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Mu Gua*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Mu Gua	G063H0424621	62085 [†]	20
PhytoComm	Mu Gua	G063H0424621	62086 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Mu Gua*.

Supplier	Substance	Batch	Spectra
Phytocomm	Mu Gua	G063H0424221	1
PhytoComm	Mu Gua	G063H0424221	1
Phytocomm	Mu Gua	G063H0424521	4

- 845 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	39	1	12 442
Type C	6	0	6	839

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	97.5000 % (> 90.0000 %)
Type C	99.5789 % (> 98.9891 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62086	62086	0.00	8.83
62085	62085	0.00	8.96

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Nü Zhen Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60065-2019-09-24
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
PhytoComm	Nü Zhen Zi	G138H0345821	62343	40	from supplier
PhytoComm	Nü Zhen Zi	G138H0345821	62344	40	from supplier
PhytoComm	Nü Zhen Zi	G138HS010SK1	62569	40	from supplier
PhytoComm	Nü Zhen Zi	G138HS010SK1	62570	40	from supplier

Validation samples

A total of 37 534 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 *Nü Zhen Zi*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Nü Zhen Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Nü Zhen Zi	G138H0345721	62213 [†]	20
PhytoComm	Nü Zhen Zi	G138H0345721	62214 [†]	20
PhytoComm	Nü Zhen Zi	G138H0345821	62343 [†]	20
PhytoComm	Nü Zhen Zi	G138H0345821	62344 [†]	20
PhytoComm	Nü Zhen Zi	G138HS010SK1	62569 [†]	20
PhytoComm	Nü Zhen Zi	G138HS010SK1	62570 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Nü Zhen Zi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Nü Zhen Zi	G138H0345421	1
Phytocomm	Nü Zhen Zi	420319901	1
PhytoComm	Nü Zhen Zi	G138H0345421	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	0	3	848

The substance/substance group *Nü Zhen 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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62570	62570	0.00	17.37
62569	62569	0.00	17.36
62344	62344	0.00	11.77
62343	62343	0.00	11.45
62213	62213	0.00	8.41
62214	62214	0.00	8.14

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Pi Pa Ye**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60201-2019-09-24
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	G099HS166RP1	62451	40	from supplier
PhytoComm	Pi Pa Ye	G099HS166RP1	62452	40	from supplier

Validation samples

A total of 37 534 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 *Pi Pa Ye*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Pi Pa Ye*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Pi Pa Ye	G099HS166RP1	62451 [†]	20
PhytoComm	Pi Pa Ye	G099HS166RP1	62452 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Pi Pa Ye*.

Supplier	Substance	Batch	Spectra
Phytocomm	Pi Pa Ye	G099H0832221	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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	2	78	2	24 119
Type B	2	33	7	12 440
Type C	0	0	1	850

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	99.9949 % (> 99.9794 %)	97.5000 % (> 93.7500 %)
Type B	99.9924 % (> 99.9621 %)	82.5000 % (> 75.0000 %)
Type C	100.0000 % (> 98.8311 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62451	62451	0.00	4.17
62452	62452	0.00	4.27

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Pu Gong Ying**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50358-2019-09-24
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
PhytoComm	Pu Gong Ying	G239HS308RN1	62263	40	from supplier
PhytoComm	Pu Gong Ying	G239HS308RN1	62264	40	from supplier
PhytoComm	Pu Gong Ying	G239HS308SH1	62635	40	from supplier
PhytoComm	Pu Gong Ying	G239HS308SH1	62636	40	from supplier

Validation samples

A total of 37 534 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 8 reference samples from the substance/substance group *Pu Gong Ying*. These samples are listed above in the [calibration samples](#) section.
- 23 881 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 160 spectra of 8 reference samples from the substance/substance group *Pu Gong Ying*.

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
PhytoComm	Pu Gong Ying	G239HS308RN1	62263 [†]	20
PhytoComm	Pu Gong Ying	G239HS308RN1	62264 [†]	20
PhytoComm	Pu Gong Ying	G239HS308SH1	62635 [†]	20
PhytoComm	Pu Gong Ying	G239HS308SH1	62636 [†]	20

- 12 322 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 4 *Apo-Ident* customers from 1 batches from the substance/substance group *Pu Gong Ying*.

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Phytocomm	Pu Gong Ying	G239H1315321	5
PhytoComm	Pu Gong Ying	G239H1315321	1

- 845 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	320	0	23 881
Type B	0	159	1	12 322
Type C	3	0	6	842

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 % (> 99.9687 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9390 %)	99.3750 % (> 97.5000 %)
Type C	99.7134 % (> 99.1236 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62264	62264	0.00	7.13
62263	62263	0.00	7.50
62635	62635	0.00	7.62

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62120	62120	0.00	18.14
62636	62636	0.00	7.82
62119	62119	0.00	18.43
62163	62163	0.00	16.96
62164	62164	0.00	17.08

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Qiang Huo**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60109-2019-09-24
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
PhytoComm	Qiang Huo	G172H0840721	62361	40	from supplier
PhytoComm	Qiang Huo	G172H0840721	62362	40	from supplier

Validation samples

A total of 37 534 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 *Qiang Huo*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Qiang Huo*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Qiang Huo	G172H0840621	62121 [†]	20
PhytoComm	Qiang Huo	G172H0840621	62122 [†]	20
PhytoComm	Qiang Huo	G172H0840721	62361 [†]	20
PhytoComm	Qiang Huo	G172H0840721	62362 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Qiang Huo*.

Supplier	Substance	Batch	Spectra
Phytocomm	Qiang Huo	g172h0841321	1
Phytocomm	Qiang Huo	G172H0840321	1
PhytoComm	Qiang Huo	G172H0840321	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	6	1	2	842

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.5885 % (> 98.9997 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62122	62122	0.00	8.60
62121	62121	0.00	9.11
62362	62362	0.00	11.85
62361	62361	0.00	11.10

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Qin Jiao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60222-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Qin Jiao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Qin Jiao	G113H1059521	61772 [†]	20
PhytoComm	Qin Jiao	G113H1059521	61814 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Qin Jiao*.

Supplier	Substance	Batch	Spectra
PhytoComm	Qin Jiao	G113H1059121	1
PhytoComm	Qin Jiao	G113H1059521	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	1	1	1	848

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.8843 % (> 99.2966 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61814	61814	0.00	12.26
61772	61772	0.00	12.12

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Qing Hao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60198-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Qing Hao; Artemisiae apiacae herba

Special notes

When selecting the *Qing 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 *Qing Hao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Qing Hao	G031H0810721	62395	40	from supplier
PhytoComm	Qing Hao	G031H0810721	62396	40	from supplier

Validation samples

A total of 37 534 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 Hao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Qing Hao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Qing Hao	G031H0810721	62395 [†]	20
PhytoComm	Qing Hao	G031H0810721	62396 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Qing Hao*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Hao* can be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

spectra of the various substances were compared with *Qing 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	80	0	24 121
Type B	0	40	0	12 442
Type C	0	0	0	851

The substance/substance group *Qing 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62396	62396	0.00	13.11
62395	62395	0.00	12.77

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Qing Pi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50371-2019-09-24
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	G074H0809821	62379	40	from supplier
PhytoComm	Qing Pi	G074H0809821	62380	40	from supplier
PhytoComm	Qing Pi	G074HS361SK1	62671	40	from supplier
PhytoComm	Qing Pi	G074HS361SK1	62672	40	from supplier

Validation samples

A total of 37 534 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 *Qing Pi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Qing Pi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Qing Pi	G074H0809821	62379 [†]	20
PhytoComm	Qing Pi	G074H0809821	62380 [†]	20
PhytoComm	Qing Pi	G074HS361SK1	62671 [†]	20
PhytoComm	Qing Pi	G074HS361SK1	62672 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Qing Pi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Qing Pi	g074h100713	1
PhytoComm	Qing Pi	G074H0809621	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	2	849

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62379	62379	0.00	11.74
62672	62672	0.00	7.87
62380	62380	0.00	12.35
62671	62671	0.00	10.05

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Rou Cong Rong**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60182-2019-09-24
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	G072HS108SG1	62667	40	from supplier
PhytoComm	Rou Cong Rong	G072HS108SG1	62668	40	from supplier

Validation samples

A total of 37 534 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 Cong Rong*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Rou Cong Rong*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Rou Cong Rong	G072HS108SG1	62667 [†]	20
PhytoComm	Rou Cong Rong	G072HS108SG1	62668 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Rou Cong Rong*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

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	80	0	24 121
Type B	0	40	0	12 442
Type C	0	0	0	851

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62668	62668	0.00	16.90
62667	62667	0.00	15.58

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Rou Gui**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60169-2019-09-24
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
PhytoComm	Rou Gui	G069HS204RN1	62271	40	from supplier
PhytoComm	Rou Gui	G069HS204RN1	62272	40	from supplier
PhytoComm	Rou Gui	G069HS204RM1	62443	40	from supplier
PhytoComm	Rou Gui	G069HS204RM1	62444	40	from supplier

Validation samples

A total of 37 534 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 *Rou Gui*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Rou Gui*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Rou Gui	G069HS204QM1	62187 [†]	20
PhytoComm	Rou Gui	G069HS204QM1	62188 [†]	20
PhytoComm	Rou Gui	G069HS204RN1	62271 [†]	20
PhytoComm	Rou Gui	G069HS204RN1	62272 [†]	20
PhytoComm	Rou Gui	G069HS204RM1	62443 [†]	20
PhytoComm	Rou Gui	G069HS204RM1	62444 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Rou Gui*.

Supplier	Substance	Batch	Spectra
Phytocomm	Rou Gui	H0617022	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
PhytoComm	Rou Gui	G069H0617123	2
Phytocomm	Rou Gui	G069H0617323	1
Phytocomm	Rou Gui	g069h0617123	1
PhytoComm	Rou Gui	G069H0617323	1

- 845 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	11	237	3	23 950
Type B	7	105	15	12 355
Type C	1	0	6	844

The substance/substance group *Rou 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	99.9632 % (> 99.9475 %)	98.7500 % (> 97.5000 %)
Type B	99.9238 % (> 99.8933 %)	87.5000 % (> 85.0000 %)
Type C	99.7685 % (> 99.1787 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62444	62444	0.00	5.51
62271	62271	0.00	3.52
62443	62443	0.00	3.65
62187	62187	0.00	3.28
62272	62272	0.00	2.87
62188	62188	0.00	3.09

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ru Xiang**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50370-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Ru Xiang*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ru Xiang	G174H0820621	61935 [†]	20
PhytoComm	Ru Xiang	G174H0820621	61936 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Ru Xiang*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ru Xiang	G174H0820231	1
Phytocomm	Ru Xiang	G174H0820421	1
PhytoComm	Ru Xiang	G174H0820421	2

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	4	847

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well 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	66.65
61936	61936	0.00	66.56

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **San Leng**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60029-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *San Leng*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	San Leng	G270H0311721	62235 [†]	20
PhytoComm	San Leng	G270H0311721	62236 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *San Leng*.

Supplier	Substance	Batch	Spectra
PhytoComm	San Leng	G270H0311221	1
Phytocomm	San Leng	g270h0311221	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	1	1	1	848

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.9074 % (> 99.3197 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62236	62236	0.00	9.47
62235	62235	0.00	9.36

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **San Qi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60415-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

San Qi; Notoginseng 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 37 534 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 [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *San Qi*.

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

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *San Qi*.

Supplier	Substance	Batch	Spectra
Phytocomm	San Qi	g203h0312021	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 041
Type B	0	80	0	12 402
Type C	1	0	1	849

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.7685 % (> 99.1841 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62245	62245	0.00	13.17
62246	62246	0.00	13.16
62136	62136	0.00	12.21
62135	62135	0.00	12.58

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Sang Bai Pi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50287-2019-09-24
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	G161H1042821	62357	40	from supplier
PhytoComm	Sang Bai Pi	G161H1042821	62358	40	from supplier
PhytoComm	Sang Bai Pi	G161H1042822	62471	40	from supplier
PhytoComm	Sang Bai Pi	G161H1042822	62472	40	from supplier

Validation samples

A total of 37 534 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 *Sang Bai Pi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Sang Bai Pi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sang Bai Pi	G161H1042821	62357 [†]	20
PhytoComm	Sang Bai Pi	G161H1042821	62358 [†]	20
PhytoComm	Sang Bai Pi	G161H1042822	62471 [†]	20
PhytoComm	Sang Bai Pi	G161H1042822	62472 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Sang Bai Pi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Sang Bai Pi	G161H1042321	1
PhytoComm	Sang Bai Pi	G161H1042321	2
PhytoComm	Sang Bai Pi	G161H1042322	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 847 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	1	0	4	846

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.7685 % (> 99.1792 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62472	62472	0.00	14.18
62357	62357	0.00	14.98
62471	62471	0.00	16.01
62358	62358	0.00	14.86

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Sang Ji Shend**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60142-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sang Ji Shend; Taxilli herba

Special notes

When selecting the *Sang Ji Shend* substance/substance group, the following information is displayed to 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 Ji Shend*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Sang Ji Shend	G146H1045821	62345	40	from supplier
PhytoComm	Sang Ji Shend	G146H1045821	62346	40	from supplier
PhytoComm	Sang Ji Shend	G146H1045822	62543	40	from supplier
PhytoComm	Sang Ji Shend	G146H1045822	62544	40	from supplier

Validation samples

A total of 37 534 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 *Sang Ji Shend*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Sang Ji Shend*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sang Ji Shend	G146H1045821	62345 [†]	20
PhytoComm	Sang Ji Shend	G146H1045821	62346 [†]	20
PhytoComm	Sang Ji Shend	G146H1045822	62543 [†]	20
PhytoComm	Sang Ji Shend	G146H1045822	62544 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Sang Ji Shend*.

Supplier	Substance	Batch	Spectra
Phytocomm	Sang Ji Shend	g146h1045222	1
PhytoComm	Sang Ji Shend	G146H1045322	1
Phytocomm	Sang Ji Shend	G146H1045522	4

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Ji Shend* 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 Ji Shend* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 041
Type B	0	80	0	12 402
Type C	1	2	4	844

The substance/substance group *Sang Ji Shend* 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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.9074 % (> 99.3176 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62543	62543	0.00	15.75
62544	62544	0.00	15.87
62345	62345	0.00	17.13
62346	62346	0.00	17.23

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Sang Ye**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60079-2019-09-24
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	G162HS206RQ1	62461	40	from supplier
PhytoComm	Sang Ye	G162HS206RQ1	62462	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Sang Ye*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sang Ye	G162HS206RQ1	62461 [†]	20
PhytoComm	Sang Ye	G162HS206RQ1	62462 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Sang Ye*.

Supplier	Substance	Batch	Spectra
Phytocomm	Sang Ye	G162H1043121	1
Phytocomm	Sang Ye	G162H1043421	4

- 846 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	1	40	0	12 441
Type C	0	0	5	846

The substance/substance group *Sang 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	99.9962 % (> 99.9659 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8208 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62461	62461	0.00	13.61
62462	62462	0.00	12.15

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Sang Zhi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60091-2019-09-24
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
PhytoComm	Sang Zhi	G164H1044721	62359	40	from supplier
PhytoComm	Sang Zhi	G164H1044721	62360	40	from supplier
PhytoComm	Sang Zhi	G164H1044821	62473	40	from supplier
PhytoComm	Sang Zhi	G164H1044821	62474	40	from supplier

Validation samples

A total of 37 534 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 *Sang Zhi*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Sang Zhi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sang Zhi	G164H1044621	61969 [†]	20
PhytoComm	Sang Zhi	G164H1044621	61970 [†]	20
PhytoComm	Sang Zhi	G164H1044721	62359 [†]	20
PhytoComm	Sang Zhi	G164H1044721	62360 [†]	20
PhytoComm	Sang Zhi	G164H1044821	62473 [†]	20
PhytoComm	Sang Zhi	G164H1044821	62474 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Sang Zhi*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *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	240	0	23 961
Type B	0	119	1	12 362
Type C	9	0	0	842

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	99.1667 % (> 96.6667 %)
Type C	98.5957 % (> 98.0048 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62360	62360	0.00	9.25
61970	61970	0.00	9.02
62473	62473	0.00	6.56
61969	61969	0.00	8.87
62359	62359	0.00	9.61
62474	62474	0.00	6.81

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Sha Ren**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60184-2019-09-24
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	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
PhytoComm	Sha Ren	G018H0939821	62401	40	from supplier
PhytoComm	Sha Ren	G018H0939821	62404	40	from supplier

Validation samples

A total of 37 534 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 *Sha Ren*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Sha Ren*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sha Ren	G018H0939523	61799 [†]	20
PhytoComm	Sha Ren	G018H0939523	61818 [†]	20
PhytoComm	Sha Ren	G018H0939622	62095 [†]	20
PhytoComm	Sha Ren	G018H0939622	62096 [†]	20
PhytoComm	Sha Ren	G018H0939821	62401 [†]	20
PhytoComm	Sha Ren	G018H0939821	62404 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Sha Ren*.

Supplier	Substance	Batch	Spectra
Euro OTC	Sha Ren	H0939022	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Phytocomm	Sha Ren	G018H0939321	1
Phytocomm	Sha Ren	g018h0939321	1
PhytoComm	Sha Ren	G018H0939523	1
Phytocomm	Sha Ren	G018H0939522	1

- 846 spectra from 12 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	2	4	1	844

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	99.8071 % (> 99.2175 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62095	62095	0.00	11.17
62404	62404	0.00	14.18
62096	62096	0.00	10.81
61799	61799	0.00	11.76
62401	62401	0.00	14.07
61818	61818	0.00	11.88

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Sha Shen (Bei)**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60200-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sha Shen (Bei); Glehniae radix

Special notes

When selecting the *Sha Shen (Bei)* substance/substance group, the following information is displayed to 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 Shen (Bei)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Sha Shen (Bei)	G117H0754821	62587	40	from supplier

Validation samples

A total of 37 534 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 *Sha Shen (Bei)*. These samples are listed above in the [calibration samples](#) section.
- 24 161 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 79 spectra of 2 reference samples from the substance/substance group *Sha Shen (Bei)*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sha Shen (Bei)	G117H0754821	62587 [†]	20
PhytoComm	Sha Shen (Bei)	G117H0754821	62588	59

- 12 403 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 3 *Apo-Ident* customers from 1 batches from the substance/substance group *Sha Shen (Bei)*.

Supplier	Substance	Batch	Spectra
Phytocomm	Sha Shen (Bei)	G117H0754322	4

- 847 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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 Shen (Bei)* 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 Shen (Bei)* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 161
Type B	0	78	1	12 403
Type C	1	0	4	846

The substance/substance group *Sha Shen (Bei)* 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 % (> 99.9692 %)	100.0000 % (> 85.0000 %)
Type B	100.0000 % (> 99.9392 %)	98.7342 % (> 94.9367 %)
Type C	99.8457 % (> 99.2564 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62587	62587	0.00	8.98

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Shan Yao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60207-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Shan Yao; Dioscoreae oppositae rhizoma

Special notes

When selecting the *Shan 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 *Shan Yao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Shan Yao	G091H0330821	62331	40	from supplier
PhytoComm	Shan Yao	G091H0330821	62332	40	from supplier
PhytoComm	Shan Yao	G091HS024RQ1	62447	40	from supplier
PhytoComm	Shan Yao	G091HS024RQ1	62448	40	from supplier
PhytoComm	Shan Yao	G091H0330822	62523	40	from supplier
PhytoComm	Shan Yao	G091H0330822	62524	40	from supplier

Validation samples

A total of 37 534 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 *Shan Yao*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Shan Yao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Shan Yao	G091H0330821	62331 [†]	20
PhytoComm	Shan Yao	G091H0330821	62332 [†]	20
PhytoComm	Shan Yao	G091HS024RQ1	62447 [†]	20
PhytoComm	Shan Yao	G091HS024RQ1	62448 [†]	20
PhytoComm	Shan Yao	G091H0330822	62523 [†]	20
PhytoComm	Shan Yao	G091H0330822	62524 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 3 *Apo-Ident* customers from 1 batches from the substance/substance group *Shan Yao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Shan Yao	G091H0330521	2
PhytoComm	Shan Yao	G091H0330521	2

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 847 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 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 *Shan 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	3	238	2	23 958
Type B	10	117	3	12 352
Type C	3	2	2	844

The substance/substance group *Shan 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	99.9822 % (> 99.9666 %)	99.1667 % (> 97.9167 %)
Type B	99.8742 % (> 99.8438 %)	97.5000 % (> 95.0000 %)
Type C	99.6528 % (> 99.0635 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62524	62524	0.00	7.32
62448	62448	0.00	4.04
62447	62447	0.00	4.00
62331	62331	0.00	8.50
62523	62523	0.00	6.89
62332	62332	0.00	9.61

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Shan Yu Rou**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60226-2019-09-24
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	G080HS027RH1	62269	40	from supplier
PhytoComm	Shan Yu Rou	G080HS027RH1	62270	40	from supplier
PhytoComm	Shan Yu Rou	G080HS027SK1	62571	40	from supplier
PhytoComm	Shan Yu Rou	G080HS027SK1	62572	40	from supplier

Validation samples

A total of 37 534 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 *Shan Yu Rou*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Shan Yu Rou*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Shan Yu Rou	G080HS027RH1	62269 [†]	20
PhytoComm	Shan Yu Rou	G080HS027RH1	62270 [†]	20
PhytoComm	Shan Yu Rou	G080HS027SK1	62571 [†]	20
PhytoComm	Shan Yu Rou	G080HS027SK1	62572 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Shan Yu Rou*.

Supplier	Substance	Batch	Spectra
Phytocomm	Shan Yu Rou	G080H0333221	1
Phytocomm	Shan Yu Rou	g080h0333221	1
Phytocomm	Shan Yu Rou	G080H0333421	1
PhytoComm	Shan Yu Rou	G080H0333621	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 847 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	1	0	4	846

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.8457 % (> 99.2564 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62572	62572	0.00	12.75
62269	62269	0.00	10.24
62571	62571	0.00	12.25
62270	62270	0.00	9.60

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **She Gan**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60335-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *She Gan*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	She Gan	G048H1034621	61771 [†]	20
PhytoComm	She Gan	G048H1034621	61828 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *She Gan*.

Supplier	Substance	Batch	Spectra
Phytocomm	She Gan	G048H1034422	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	12	0	1	838

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	98.9141 % (> 98.3297 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well 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	5.12
61828	61828	0.00	5.33

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Shen Qu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60020-2019-09-24
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	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
PhytoComm	Shen Qu	G156HS222RP1	62459	40	from supplier
PhytoComm	Shen Qu	G156HS222RP1	62460	40	from supplier
PhytoComm	Shen Qu	G156H0935821	62467	40	from supplier
PhytoComm	Shen Qu	G156H0935821	62468	40	from supplier

Validation samples

A total of 37 534 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 8 reference samples from the substance/substance group *Shen Qu*. These samples are listed above in the [calibration samples](#) section.
- 23 881 spectra from a total of 293 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 160 spectra of 8 reference samples from the substance/substance group *Shen Qu*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Shen Qu	G156H0935522	61971 [†]	20
PhytoComm	Shen Qu	G156H0935522	61972 [†]	20
PhytoComm	Shen Qu	G156H0935621	62259 [†]	20
PhytoComm	Shen Qu	G156H0935621	62260 [†]	20
PhytoComm	Shen Qu	G156HS222RP1	62459 [†]	20
PhytoComm	Shen Qu	G156HS222RP1	62460 [†]	20
PhytoComm	Shen Qu	G156H0935821	62467 [†]	20
PhytoComm	Shen Qu	G156H0935821	62468 [†]	20

- 12 322 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Shen Qu*.

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
PhytoComm	Shen Qu	G156H0935121	1
phytocomm	Shen Qu	g156h0935421	1
PhytoComm	Shen Qu	G156H0935521	1
PhytoComm	Shen Qu	G156H0935521	1
PhytoComm	Shen Qu	G156H0935522	1

- 846 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	320	0	23 881
Type B	0	159	1	12 322
Type C	1	2	3	845

The substance/substance group *Shen Qu* 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 % (> 99.9687 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9390 %)	99.3750 % (> 97.5000 %)
Type C	99.9074 % (> 99.3178 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
61972	61972	0.00	24.20
62460	62460	0.00	6.14
62459	62459	0.00	5.95
62259	62259	0.00	25.97
62468	62468	0.00	16.57
61971	61971	0.00	23.91
62467	62467	0.00	16.62
62260	62260	0.00	25.42

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Sheng Jiang**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60017-2019-09-24
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	G253H0534623	62141	40	from supplier
PhytoComm	Sheng Jiang	G253H0534623	62142	40	from supplier
PhytoComm	Sheng Jiang	G253HS085SK1	62549	40	from supplier
PhytoComm	Sheng Jiang	G253HS085SK1	62550	40	from supplier

Validation samples

A total of 37 534 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 Jiang*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Sheng Jiang*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sheng Jiang	G253H0534623	62141 [†]	20
PhytoComm	Sheng Jiang	G253H0534623	62142 [†]	20
PhytoComm	Sheng Jiang	G253HS085SK1	62549 [†]	20
PhytoComm	Sheng Jiang	G253HS085SK1	62550 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Sheng Jiang*.

Supplier	Substance	Batch	Spectra
Phytocomm	Sheng Jiang	G253H0534221	1
PhytoComm	Sheng Jiang	G253H0534321	1
Phytocomm	Sheng Jiang	G253H0534522	1
PhytoComm	Sheng Jiang	G253H0534522	3

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	6	149	11	24 035
Type B	19	70	10	12 383
Type C	1	0	6	844

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	99.9771 % (> 99.9615 %)	93.1250 % (> 91.2500 %)
Type B	99.8385 % (> 99.8081 %)	87.5000 % (> 83.7500 %)
Type C	99.8843 % (> 99.2944 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62549	62549	0.00	2.41
62550	62550	0.00	2.96
62141	62141	0.00	10.42
62142	62142	0.00	8.86

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Sheng Ma**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60216-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Sheng Ma*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Sheng Ma	G068H0437621	62079 [†]	20
PhytoComm	Sheng Ma	G068H0437621	62080 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Sheng Ma*.

Supplier	Substance	Batch	Spectra
Phytocomm	Sheng Ma	g068h04317121	1
Phytocomm	Sheng Ma	G068H0437421	2

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	3	0	3	845

The substance/substance group *Sheng Ma* 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.7685 % (> 99.1798 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well 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	8.45
62080	62080	0.00	8.17

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Shi Gao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50368-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Shi Gao; Gypsum fibrosum

Special notes

When selecting the *Shi Gao* substance/substance group, the following information is displayed to 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 Gao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Shi Gao	G120HS081SH1	62561	40	from supplier
PhytoComm	Shi Gao	G120HS081SH1	62562	40	from supplier

Validation samples

A total of 37 534 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 Gao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 130 spectra of 4 reference samples from the substance/substance group *Shi Gao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Shi Gao	G120H0541721	62229	45
PhytoComm	Shi Gao	G120H0541721	62230	45
PhytoComm	Shi Gao	G120HS081SH1	62561 [†]	20
PhytoComm	Shi Gao	G120HS081SH1	62562 [†]	20

- 12 352 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 1 batches from the substance/substance group *Shi Gao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Shi Gao	G120H0541223	1
PhytoComm	Shi Gao	G120H0541223	2

- 848 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Gao* 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 Gao* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 121
Type B	0	40	90	12 352
Type C	0	0	3	848

The substance/substance group *Shi Gao* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9390 %)	30.7692 % (> 28.4615 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62561	62561	0.00	54.88
62562	62562	0.00	54.42

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Shu Di (Huang)**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60006-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Shu Di (Huang); 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)	G210H1601822	62297	40	from supplier
PhytoComm	Shu Di (Huang)	G210H1601822	62298	40	from supplier
PhytoComm	Shu Di (Huang)	G210H1601823	62493	40	from supplier
PhytoComm	Shu Di (Huang)	G210H1601823	62494	40	from supplier

Validation samples

A total of 37 534 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 *Shu Di (Huang)*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Shu Di (Huang)*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Shu Di (Huang)	G210H1601822	62297 [†]	20
PhytoComm	Shu Di (Huang)	G210H1601822	62298 [†]	20
PhytoComm	Shu Di (Huang)	G210H1601823	62493 [†]	20
PhytoComm	Shu Di (Huang)	G210H1601823	62494 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Shu Di (Huang)*.

Supplier	Substance	Batch	Spectra
PhytoComm	Shu Di (Huang)	G210H1601121	1
Phytocomm	Shu Di (Huang)	G210H1601221	1
Hedinger	Shu Di (Huang)	g210h1601221	4
Phytocomm	Shu Di (Huang)	G210H1601421	6
Phytocomm	Shu Di (Huang)	G210H1601521	3

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 836 spectra from 12 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	6	0	15	830

The substance/substance group *Shu Di (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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.4599 % (> 98.8694 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62493	62493	0.00	17.92
62298	62298	0.00	24.00
62297	62297	0.00	24.31
62494	62494	0.00	17.87

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Suan Zao Ren**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60059-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Suan Zao Ren*.

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

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Suan Zao Ren*.

Supplier	Substance	Batch	Spectra
Phytocomm	Suan Zao Ren	g254h1418121	2
Phytocomm	Suan Zao Ren	G254H1418421	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 041
Type B	0	80	0	12 402
Type C	0	0	3	848

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62133	62133	0.00	20.91
61894	61894	0.00	19.35
62134	62134	0.00	21.98
61893	61893	0.00	20.26

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Tai Zi Shen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60114-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tai Zi Shen; Pseudostellariae heterophyllae radix

Special notes

When selecting the *Tai Zi 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 *Tai Zi Shen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Tai Zi Shen	G204H0446721	62299	40	from supplier
PhytoComm	Tai Zi Shen	G204H0446721	62300	40	from supplier
PhytoComm	Tai Zi Shen	G204HM066SK1	62595	40	from supplier
PhytoComm	Tai Zi Shen	G204HM066SK1	62596	40	from supplier

Validation samples

A total of 37 534 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 *Tai Zi Shen*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Tai Zi Shen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Tai Zi Shen	G204H0446721	62299 [†]	20
PhytoComm	Tai Zi Shen	G204H0446721	62300 [†]	20
PhytoComm	Tai Zi Shen	G204HM066SK1	62595 [†]	20
PhytoComm	Tai Zi Shen	G204HM066SK1	62596 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Tai Zi Shen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Tai Zi Shen	G204H0446221	1
Phytocomm	Tai Zi Shen	G204H0446521	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tai Zi 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 *Tai Zi 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	1	160	0	24 040
Type B	0	78	2	12 402
Type C	1	1	1	848

The substance/substance group *Tai Zi 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	99.9983 % (> 99.9827 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	97.5000 % (> 93.7500 %)
Type C	99.8843 % (> 99.2966 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62300	62300	0.00	5.14
62299	62299	0.00	5.51
62596	62596	0.00	5.41
62595	62595	0.00	5.78

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Tao Ren**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60454-2019-09-24
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	G184HS220SK1	62609	40	from supplier
PhytoComm	Tao Ren	G184HS220SK1	62610	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Tao Ren*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Tao Ren	G184HS220SK1	62609 [†]	20
PhytoComm	Tao Ren	G184HS220SK1	62610 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Tao Ren*.

Supplier	Substance	Batch	Spectra
Phytocomm	Tao Ren	g184h1007122	1
PhytoComm	Tao Ren	G184H1007321	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	2	77	3	24 119
Type B	0	29	11	12 442
Type C	0	0	2	849

The substance/substance group *Tao 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	99.9924 % (> 99.9768 %)	96.2500 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	72.5000 % (> 65.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62609	62609	0.00	3.99
62610	62610	0.00	4.15

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Tian Hua Fen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60139-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tian Hua Fen; Trichosanthis radix

Special notes

When selecting the *Tian Hua Fen* substance/substance group, the following information is displayed to 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 *Tian Hua Fen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Tian Hua Fen	G242H0417821	62315	40	from supplier
PhytoComm	Tian Hua Fen	G242H0417821	62316	40	from supplier
PhytoComm	Tian Hua Fen	G242HS040SG1	62633	40	from supplier
PhytoComm	Tian Hua Fen	G242HS040SG1	62634	40	from supplier

Validation samples

A total of 37 534 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 *Tian Hua Fen*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Tian Hua Fen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Tian Hua Fen	G242H0417821	62315 [†]	20
PhytoComm	Tian Hua Fen	G242H0417821	62316 [†]	20
PhytoComm	Tian Hua Fen	G242HS040SG1	62633 [†]	20
PhytoComm	Tian Hua Fen	G242HS040SG1	62634 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Tian Hua Fen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Tian Hua Fen	h0417022	1
Phytocomm	Tian Hua Fen	G242H0417423	2
Phytocomm	Tian Hua Fen	G242H0417522	1
PhytoComm	Tian Hua Fen	G242H0417522	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 846 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tian Hua Fen* 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 *Tian Hua Fen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 041
Type B	0	80	0	12 402
Type C	0	0	5	846

The substance/substance group *Tian Hua Fen* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8208 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62316	62316	0.00	9.14
62633	62633	0.00	7.13
62634	62634	0.00	6.96
62315	62315	0.00	9.16

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Tian Men Dong**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60156-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Tian Men Dong; Asparagi cochinensis radix

Special notes

When selecting the *Tian 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 *Tian Men Dong*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Tian Men Dong	G037HS041RR1	62437	40	from supplier
PhytoComm	Tian Men Dong	G037HS041RR1	62438	40	from supplier

Validation samples

A total of 37 534 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 *Tian Men Dong*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Tian Men Dong*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Tian Men Dong	G037HS041RR1	62437 [†]	20
PhytoComm	Tian Men Dong	G037HS041RR1	62438 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Tian Men Dong*.

Supplier	Substance	Batch	Spectra
Phytocomm	Tian Men Dong	g03h0415521	1
Phytocomm	Tian Men Dong	G037H0415221	1
Phytocomm	Tian Men Dong	g037h0415221	1
Phytocomm	Tian Men Dong	G037H0415321	1

- 847 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tian 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 *Tian 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	80	0	24 121
Type B	0	39	1	12 442
Type C	0	0	4	847

The substance/substance group *Tian 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	97.5000 % (> 90.0000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62438	62438	0.00	7.13
62437	62437	0.00	7.32

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Tu Fu Ling**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50885-2019-09-24
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
PhytoComm	Tu Fu Ling	G231HS009RK1	62427	40	from supplier
PhytoComm	Tu Fu Ling	G231HS009RK1	62428	40	from supplier
PhytoComm	Tu Fu Ling	G231HS009SK1	62641	40	from supplier
PhytoComm	Tu Fu Ling	G231HS009SK1	62642	40	from supplier

Validation samples

A total of 37 534 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 *Tu Fu Ling*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Tu Fu Ling*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Tu Fu Ling	G231H0325621	61915 [†]	20
PhytoComm	Tu Fu Ling	G231H0325621	61916 [†]	20
PhytoComm	Tu Fu Ling	G231HS009RK1	62427 [†]	20
PhytoComm	Tu Fu Ling	G231HS009RK1	62428 [†]	20
PhytoComm	Tu Fu Ling	G231HS009SK1	62641 [†]	20
PhytoComm	Tu Fu Ling	G231HS009SK1	62642 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Tu Fu Ling*.

Supplier	Substance	Batch	Spectra
Phytocomm	Tu Fu Ling	G231H0325121	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
PhytoComm	Tu Fu Ling	G231H0325121	1
PhytoComm	Tu Fu Ling	G23H0325121	1
Phytocomm	Tu Fu Ling	G231H0325421	2
PhytoComm	Tu Fu Ling	G231H0325421	1

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	118	2	12 362
Type C	1	1	5	844

The substance/substance group *Tu 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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	98.3333 % (> 95.8333 %)
Type C	99.8843 % (> 99.2944 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62641	62641	0.00	8.06
62642	62642	0.00	9.58
61916	61916	0.00	14.45
62427	62427	0.00	5.53
61915	61915	0.00	14.64
62428	62428	0.00	6.97

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Tu Si Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60217-2019-09-24
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	G086H1243823	62521	40	from supplier
PhytoComm	Tu Si Zi	G086H1243823	62522	40	from supplier

Validation samples

A total of 37 534 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 Si Zi*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Tu Si Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Tu Si Zi	G086H1243823	62521 [†]	20
PhytoComm	Tu Si Zi	G086H1243823	62522 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Tu Si Zi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Tu Si Zi	h1243022	1
Phytocomm	Tu Si Zi	G086H1243521	3
PhytoComm	Tu Si Zi	G086H1243521	1

- 846 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	40	0	12 442
Type C	0	0	5	846

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8208 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62522	62522	0.00	25.11
62521	62521	0.00	25.43

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Wang Bu Liu Xing**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50390-2019-09-24
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
PhytoComm	Wang Bu Liu Xing	G281H0456821	62463	40	from supplier
PhytoComm	Wang Bu Liu Xing	G281H0456821	62464	40	from supplier

Validation samples

A total of 37 534 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 *Wang Bu Liu Xing*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Wang Bu Liu Xing*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wang Bu Liu Xing	G281HS057QM1	62181 [†]	20
PhytoComm	Wang Bu Liu Xing	G281HS057QM1	62182 [†]	20
PhytoComm	Wang Bu Liu Xing	G281H0456821	62463 [†]	20
PhytoComm	Wang Bu Liu Xing	G281H0456821	62464 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Wang Bu Liu Xing*.

Supplier	Substance	Batch	Spectra
PhytoComm	Wang Bu Liu Xing	G281H0456322	1
PhytoComm	Wang Bu Liu Xing	G281H456421	1
Phytocomm	Wang Bu Liu Xing	G281H0456521	1
PhytoComm	Wang Bu Liu Xing	G281H0456221	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 847 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	4	847

The substance/substance group *Wang Bu Liu Xing* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8214 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62182	62182	0.00	6.34
62464	62464	0.00	22.23
62463	62463	0.00	22.77
62181	62181	0.00	7.56

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Wei Ling Xian**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60543-2019-09-24
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	G075H0943822	62381	40	from supplier
PhytoComm	Wei Ling Xian	G075H0943822	62382	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Wei Ling Xian*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wei Ling Xian	G075H0943822	62381 [†]	20
PhytoComm	Wei Ling Xian	G075H0943822	62382 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Wei Ling Xian*.

Supplier	Substance	Batch	Spectra
Phytocomm	Wei Ling Xian	G075H0943223	1
PhytoComm	Wei Ling Xian	G075H0943223	2
PhytoComm	Wei Ling Xian	G075H0943223	1
Phytocomm	Wei Ling Xian	G075H0943223	1
Phytocomm	Wei Ling Xian	G075H0943422	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 845 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	6	845

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8204 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62381	62381	0.00	15.52
62382	62382	0.00	15.53

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Wu Mei**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60021-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Wu Mei; Pruni mume fructus

Special notes

When selecting the *Wu Mei* substance/substance group, the following information is displayed to 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 Mei*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Wu Mei	G167H1026821	62477	40	from supplier
PhytoComm	Wu Mei	G167H1026821	62478	40	from supplier

Validation samples

A total of 37 534 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 Mei*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Wu Mei*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wu Mei	G167H1026821	62477 [†]	20
PhytoComm	Wu Mei	G167H1026821	62478 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Wu Mei*.

Supplier	Substance	Batch	Spectra
PhytoComm	Wu Mei	G167H1026221	1
PhytoComm	Wu Mei	G167H1026421	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Mei* 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 Mei* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 121
Type B	0	40	0	12 442
Type C	0	0	2	849

The substance/substance group *Wu Mei* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62478	62478	0.00	30.97
62477	62477	0.00	31.97

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Wu Wei Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60001-2019-09-24
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	G220HS048RP1	62265	40	from supplier
PhytoComm	Wu Wei Zi	G220HS048RP1	62266	40	from supplier
PhytoComm	Wu Wei Zi	G220HS048SK1	62551	40	from supplier
PhytoComm	Wu Wei Zi	G220HS048SK1	62552	40	from supplier

Validation samples

A total of 37 534 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 Wei Zi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Wu Wei Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wu Wei Zi	G220HS048RP1	62265 [†]	20
PhytoComm	Wu Wei Zi	G220HS048RP1	62266 [†]	20
PhytoComm	Wu Wei Zi	G220HS048SK1	62551 [†]	20
PhytoComm	Wu Wei Zi	G220HS048SK1	62552 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Wu Wei Zi*.

Supplier	Substance	Batch	Spectra
Caelo	Wu Wei Zi	G220H0401421	2
Phytocomm	Wu Wei Zi	G220H0401421	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	3	848

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62266	62266	0.00	14.60
62552	62552	0.00	10.34
62265	62265	0.00	16.55
62551	62551	0.00	10.76

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Wu Yao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60040-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Wu Yao; Linderæ 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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Wu Yao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Wu Yao	G140H1025721	62233 [†]	20
PhytoComm	Wu Yao	G140H1025721	62234 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Wu Yao*.

Supplier	Substance	Batch	Spectra
PhytoComm	Wu Yao	G140H1025221	2
Phytocomm	Wu Yao	G140H1025521	2
Phytocomm	Wu Yao	g140h1025221	1
PhytoComm	Wu Yao	G140H1025521	1

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	8	3	3	837

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	99.3441 % (> 98.7543 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62234	62234	0.00	14.39
62233	62233	0.00	14.76

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Xi Xian Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60103-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Xi Xian Cao; Siegesbeckiae herba

Special notes

When selecting the *Xi Xian 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 *Xi Xian Cao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xi Xian Cao	G229HS309SK1	62555	40	from supplier
PhytoComm	Xi Xian Cao	G229HS309SK1	62556	40	from supplier

Validation samples

A total of 37 534 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 Xian Cao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Xi Xian Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xi Xian Cao	G229HS309SK1	62555 [†]	20
PhytoComm	Xi Xian Cao	G229HS309SK1	62556 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Xi Xian Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Xi Xian Cao	G229H1431321	1
PhytoComm	Xi Xian Cao	G229H1431321	1
PhytoComm	Xi Xian Cao	G229H1431521	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Xian 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 *Xi Xian 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	24 121
Type B	0	40	0	12 442
Type C	0	0	3	848

The substance/substance group *Xi Xian 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62556	62556	0.00	8.51
62555	62555	0.00	7.76

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Xi Yang Shen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60422-2019-09-24
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	G324H0647721	62323	40	from supplier
PhytoComm	Xi Yang Shen	G324H0647721	62324	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Xi Yang Shen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xi Yang Shen	G324H0647721	62323 [†]	20
PhytoComm	Xi Yang Shen	G324H0647721	62324 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Xi Yang Shen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Xi Yang Shen	g324h0647321	1
Phytocomm	Xi Yang Shen	G324H0647321	1
Phytocomm	Xi Yang Shen	G324HS4070L1	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	3	848

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62324	62324	0.00	31.50
62323	62323	0.00	31.48

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Xia Ku Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60080-2019-09-24
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
PhytoComm	Xia Ku Cao	G202HS232RM1	62283	40	from supplier
PhytoComm	Xia Ku Cao	G202HS232RM1	62284	40	from supplier

Validation samples

A total of 37 534 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 *Xia Ku Cao*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Xia Ku Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xia Ku Cao	G202HS232QM1	62191 [†]	20
PhytoComm	Xia Ku Cao	G202HS232QM1	62192 [†]	20
PhytoComm	Xia Ku Cao	G202HS232RM1	62283 [†]	20
PhytoComm	Xia Ku Cao	G202HS232RM1	62284 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Xia Ku Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Xia Ku Cao	G202H1064221	2
PhytoComm	Xia Ku Cao	G202H1064221	2
Phytocomm	Xia Ku Cao	g202h1064121	1
Phytocomm	Xia Ku Cao	G202H1064421	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	6	845

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8204 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62283	62283	0.00	8.46
62284	62284	0.00	8.85
62192	62192	0.00	11.45
62191	62191	0.00	11.49

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Xian He Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60591-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Xian He Cao; Agrimoniae herba

Special notes

When selecting the *Xian He 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 *Xian He Cao*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xian He Cao	G008H0547921	62585	40	from supplier
PhytoComm	Xian He Cao	G008H0547921	62586	40	from supplier

Validation samples

A total of 37 534 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 *Xian He Cao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Xian He Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xian He Cao	G008H0547921	62585 [†]	20
PhytoComm	Xian He Cao	G008H0547921	62586 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Xian He Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Xian He Cao	G008H0547121	1
Phytocomm	Xian He Cao	G008H0547321	1
phytocomm	Xian He Cao	g008h0547321	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Xian He 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 *Xian He 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	24 121
Type B	0	40	0	12 442
Type C	0	0	3	848

The substance/substance group *Xian He 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62586	62586	0.00	14.51
62585	62585	0.00	16.06

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Xiang Fu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60185-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Xiang Fu; Cyperi rotundi rhizoma

Special notes

When selecting the *Xiang Fu* substance/substance group, the following information is displayed to 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 *Xiang Fu*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Xiang Fu	G088H0930821	62333	40	from supplier
PhytoComm	Xiang Fu	G088H0930821	62334	40	from supplier

Validation samples

A total of 37 534 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 *Xiang Fu*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Xiang Fu*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xiang Fu	G088H0930821	62333 [†]	20
PhytoComm	Xiang Fu	G088H0930821	62334 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 5 *Apo-Ident* customers from 3 batches from the substance/substance group *Xiang Fu*.

Supplier	Substance	Batch	Spectra
PhytoComm	Xiang Fu	G088H0930321	1
Phytocomm	Xiang Fu	g088h0930123	1
Phytocomm	Xiang Fu	G088H0930521	5
PhytoComm	Xiang Fu	G088H0930521	1

- 843 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Xiang Fu* 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 *Xiang Fu* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 121
Type B	0	40	0	12 442
Type C	0	5	3	843

The substance/substance group *Xiang Fu* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8198 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62334	62334	0.00	8.80
62333	62333	0.00	8.93

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Xie Bai**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60362-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Xie Bai; Allii bulbosus

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	G504H1830821	62321	40	from supplier
PhytoComm	Xie Bai	G504H1830821	62322	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Xie Bai*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xie Bai	G504H1830821	62321 [†]	20
PhytoComm	Xie Bai	G504H1830821	62322 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Xie Bai*.

Supplier	Substance	Batch	Spectra
PhytoComm	Xie Bai	G504H1830321	1
Phytocomm	Xie Bai	G504H1830422	1
Phytocomm	Xie Bai	G504H1830421	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	0	0	3	848

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62321	62321	0.00	11.98
62322	62322	0.00	11.77

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Xin Yi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60231-2019-09-24
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	G153H0758821	62351	40	from supplier
PhytoComm	Xin Yi	G153H0758821	62352	40	from supplier
PhytoComm	Xin Yi	G153HS139SH1	62603	40	from supplier
PhytoComm	Xin Yi	G153HS139SH1	62604	40	from supplier

Validation samples

A total of 37 534 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 *Xin Yi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Xin Yi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xin Yi	G153H0758821	62351 [†]	20
PhytoComm	Xin Yi	G153H0758821	62352 [†]	20
PhytoComm	Xin Yi	G153HS139SH1	62603 [†]	20
PhytoComm	Xin Yi	G153HS139SH1	62604 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Xin Yi*.

Supplier	Substance	Batch	Spectra
PhytoComm	Xin Yi	G153H0758321	1
Phytocomm	Xin Yi	G153H0758521	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	2	849

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62603	62603	0.00	6.47
62351	62351	0.00	21.16
62352	62352	0.00	20.31
62604	62604	0.00	6.41

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Xu Duan**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60245-2019-09-24
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	G092H2106821	62329	40	from supplier
PhytoComm	Xu Duan	G092H2106821	62330	40	from supplier
PhytoComm	Xu Duan	G092H2106822	62525	40	from supplier
PhytoComm	Xu Duan	G092H2106822	62526	40	from supplier

Validation samples

A total of 37 534 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 *Xu Duan*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Xu Duan*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xu Duan	G092H2106821	62329 [†]	20
PhytoComm	Xu Duan	G092H2106821	62330 [†]	20
PhytoComm	Xu Duan	G092H2106822	62525 [†]	20
PhytoComm	Xu Duan	G092H2106822	62526 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Xu Duan*.

Supplier	Substance	Batch	Spectra
Phytocomm	Xu Duan	G092H2106422	1

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	5	1	0	845

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	98.9198 % (> 98.3353 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62526	62526	0.00	14.27
62330	62330	0.00	11.94
62329	62329	0.00	11.34
62525	62525	0.00	14.47

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Xuan Shen**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60095-2019-09-24
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	G223HS092RN1	62273	40	from supplier
PhytoComm	Xuan Shen	G223HS092RN1	62274	40	from supplier
PhytoComm	Xuan Shen	G223HS092SH1	62553	40	from supplier
PhytoComm	Xuan Shen	G223HS092SH1	62554	40	from supplier

Validation samples

A total of 37 534 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 *Xuan Shen*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Xuan Shen*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Xuan Shen	G223HS092QH1	62199 [†]	20
PhytoComm	Xuan Shen	G223HS092QH1	62200 [†]	20
PhytoComm	Xuan Shen	G223HS092RN1	62273 [†]	20
PhytoComm	Xuan Shen	G223HS092RN1	62274 [†]	20
PhytoComm	Xuan Shen	G223HS092SH1	62553 [†]	20
PhytoComm	Xuan Shen	G223HS092SH1	62554 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Xuan Shen*.

Supplier	Substance	Batch	Spectra
Phytocomm	Xuan Shen	g22h0537322	1
Phytocomm	Xuan Shen	G223H0537421	1
Euro OTC	Xuan Shen	H0537021	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 848 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	0	3	848

The substance/substance group *Xuan 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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62200	62200	0.00	19.32
62274	62274	0.00	25.02
62273	62273	0.00	25.30
62553	62553	0.00	16.62
62554	62554	0.00	16.84
62199	62199	0.00	17.86

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yan Hu Suo**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60439-2019-09-24
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	G081H0805821	62371	40	from supplier
PhytoComm	Yan Hu Suo	G081H0805821	62372	40	from supplier
PhytoComm	Yan Hu Suo	G081HS161SG1	62677	40	from supplier
PhytoComm	Yan Hu Suo	G081HS161SG1	62678	40	from supplier

Validation samples

A total of 37 534 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 *Yan Hu Suo*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Yan Hu Suo*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yan Hu Suo	G081H0805821	62371 [†]	20
PhytoComm	Yan Hu Suo	G081H0805821	62372 [†]	20
PhytoComm	Yan Hu Suo	G081HS161SG1	62677 [†]	20
PhytoComm	Yan Hu Suo	G081HS161SG1	62678 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Yan Hu Suo*.

Supplier	Substance	Batch	Spectra
PhytoComm	Yan Hu Suo	G081H0805223	1
Phytocomm	Yan Hu Suo	G081H0805223	1
PhytoComm	Yan Hu Suo	G081H0805223	1
Phytocomm	Yan Hu Suo	g081f1000301	1
Phytocomm	Yan Hu Suo	G081H0805521	1
PhytoComm	Yan Hu Suo	G081H0805521	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 845 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	6	845

The substance/substance group *Yan Hu Suo* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8204 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62677	62677	0.00	7.33
62678	62678	0.00	6.61
62372	62372	0.00	10.88
62371	62371	0.00	10.72

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ye Jiao Teng**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60068-2019-09-24
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	G288H0885621	62131	40	from supplier
PhytoComm	Ye Jiao Teng	G288H0885621	62132	40	from supplier
PhytoComm	Ye Jiao Teng	G288HS163RM1	62421	40	from supplier
PhytoComm	Ye Jiao Teng	G288HS163RM1	62422	40	from supplier
PhytoComm	Ye Jiao Teng	G288HS163SK1	62625	40	from supplier
PhytoComm	Ye Jiao Teng	G288HS163SK1	62626	40	from supplier

Validation samples

A total of 37 534 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 *Ye Jiao Teng*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Ye Jiao Teng*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ye Jiao Teng	G288H0885621	62131 [†]	20
PhytoComm	Ye Jiao Teng	G288H0885621	62132 [†]	20
PhytoComm	Ye Jiao Teng	G288HS163RM1	62421 [†]	20
PhytoComm	Ye Jiao Teng	G288HS163RM1	62422 [†]	20
PhytoComm	Ye Jiao Teng	G288HS163SK1	62625 [†]	20
PhytoComm	Ye Jiao Teng	G288HS163SK1	62626 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Ye Jiao Teng*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ye Jiao Teng	G288H0885522	2

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Phytocomm	Ye Jiao Teng	g228h0085223	1
Phytocomm	Ye Jiao Teng	G288H0885223	1
PhytoComm	Ye Jiao Teng	G288H0885522	2

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	3	235	5	23 958
Type B	0	115	5	12 362
Type C	1	0	6	844

The substance/substance group *Ye Jiao Teng* 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	99.9771 % (> 99.9615 %)	97.9167 % (> 96.6667 %)
Type B	100.0000 % (> 99.9391 %)	95.8333 % (> 93.3333 %)
Type C	99.9228 % (> 99.3330 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62625	62625	0.00	7.34

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62132	62132	0.00	40.10
62626	62626	0.00	7.05
62422	62422	0.00	5.21
62131	62131	0.00	40.29
62421	62421	0.00	4.91

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yi Mu Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60105-2019-09-24
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	G134H1050621	61983	40	from supplier
PhytoComm	Yi Mu Cao	G134H1050621	61984	40	from supplier
PhytoComm	Yi Mu Cao	G134H1050821	62409	40	from supplier
PhytoComm	Yi Mu Cao	G134H1050821	62410	40	from supplier
PhytoComm	Yi Mu Cao	G134H1050822	62541	40	from supplier
PhytoComm	Yi Mu Cao	G134H1050822	62542	40	from supplier

Validation samples

A total of 37 534 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 *Yi Mu Cao*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Yi Mu Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yi Mu Cao	G134H1050621	61983 [†]	20
PhytoComm	Yi Mu Cao	G134H1050621	61984 [†]	20
PhytoComm	Yi Mu Cao	G134H1050821	62409 [†]	20
PhytoComm	Yi Mu Cao	G134H1050821	62410 [†]	20
PhytoComm	Yi Mu Cao	G134H1050822	62541 [†]	20
PhytoComm	Yi Mu Cao	G134H1050822	62542 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 7 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Yi Mu Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Yi Mu Cao	g134h1050024	1

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[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

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Supplier	Substance	Batch	Spectra
PhytoComm	Yi Mu Cao	G134H1050321	1
PhytoComm	Yi Mu Cao	G134H1050521	1
PhytoComm	Yi Mu Cao	G134H1050521	3
PhytoComm	Yi Mu Cao	G134H1050621	1

- 844 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	1	1	6	843

The substance/substance group *Yi Mu 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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	99.9228 % (> 99.3329 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62410	62410	0.00	12.88
62542	62542	0.00	15.95
61984	61984	0.00	10.21
62541	62541	0.00	15.50
62409	62409	0.00	12.92
61983	61983	0.00	9.45

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yi Yi Ren**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60174-2019-09-24
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	G078H1701622	62097	40	from supplier
PhytoComm	Yi Yi Ren	G078H1701622	62098	40	from supplier
PhytoComm	Yi Yi Ren	G078HS336RL1	62279	40	from supplier
PhytoComm	Yi Yi Ren	G078HS336RL1	62280	40	from supplier
PhytoComm	Yi Yi Ren	G078HS336SH1	62675	40	from supplier
PhytoComm	Yi Yi Ren	G078HS336SH1	62676	40	from supplier

Validation samples

A total of 37 534 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 *Yi Yi Ren*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Yi Yi Ren*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yi Yi Ren	G078H1701622	62097 [†]	20
PhytoComm	Yi Yi Ren	G078H1701622	62098 [†]	20
PhytoComm	Yi Yi Ren	G078HS336RL1	62279 [†]	20
PhytoComm	Yi Yi Ren	G078HS336RL1	62280 [†]	20
PhytoComm	Yi Yi Ren	G078HS336SH1	62675 [†]	20
PhytoComm	Yi Yi Ren	G078HS336SH1	62676 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 11 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Yi Yi Ren*.

Supplier	Substance	Batch	Spectra
Phytocomm	Yi Yi Ren	G078H1701323	1

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[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

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Supplier	Substance	Batch	Spectra
PhytoComm	Yi Yi Ren	G078H1701323	6
Phytocomm	Yi Yi Ren	g078h1701323	1
Phytocomm	Yi Yi Ren	G078H1701522	3

- 840 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	15	232	8	23 946
Type B	16	116	4	12 346
Type C	0	8	3	840

The substance/substance group *Yi Yi 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	99.9555 % (> 99.9399 %)	96.6667 % (> 95.4167 %)
Type B	99.9085 % (> 99.8781 %)	96.6667 % (> 94.1667 %)
Type C	100.0000 % (> 98.8194 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62676	62676	0.00	2.22

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62098	62098	0.00	47.32
62675	62675	0.00	2.41
62097	62097	0.00	46.62
62280	62280	0.00	3.79
62279	62279	0.00	3.03

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yi Zhi Ren**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60172-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Yi Zhi Ren; 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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Yi Zhi Ren*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yi Zhi Ren	G015H1051522	62185 [†]	20
PhytoComm	Yi Zhi Ren	G015H1051522	62186 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Yi Zhi Ren*.

Supplier	Substance	Batch	Spectra
Phytocomm	Yi Zhi Ren	G015H1051321	1
Phytocomm	Yi Zhi Ren	G015H1051521	1
PhytoComm	Yi Zhi Ren	G015H1051321	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	1	40	0	12 441
Type C	0	3	0	848

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	99.9923 % (> 99.9620 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well 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	13.52
62186	62186	0.00	13.99

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yin Chen Hao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60163-2019-09-24
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
PhytoComm	Yin Chen Hao	G034H1030721	62397	40	from supplier
PhytoComm	Yin Chen Hao	G034H1030721	62398	40	from supplier

Validation samples

A total of 37 534 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 *Yin Chen Hao*. These samples are listed above in the [calibration samples](#) section.
- 24 081 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 3 reference samples from the substance/substance group *Yin Chen Hao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yin Chen Hao	G034H1030621	61832 [†]	20
PhytoComm	Yin Chen Hao	G034H1030721	62397 [†]	20
PhytoComm	Yin Chen Hao	G034H1030721	62398 [†]	20

- 12 422 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Yin Chen Hao*.

Supplier	Substance	Batch	Spectra
Fagron	Yin Chen Hao	G034H1030421	2

- 849 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	2	120	0	24 079
Type B	9	60	0	12 413
Type C	3	0	2	846

The substance/substance group *Yin Chen Hao* 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	99.9924 % (> 99.9768 %)	100.0000 % (> 95.0000 %)
Type B	99.9314 % (> 99.9010 %)	100.0000 % (> 90.0000 %)
Type C	99.7222 % (> 99.1346 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62398	62398	0.00	11.60
62397	62397	0.00	11.11
61832	61832	0.00	7.30

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yin Yang Huo**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60228-2019-09-24
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	G098H1114622	62221	40	from supplier
PhytoComm	Yin Yang Huo	G098H1114622	62222	40	from supplier
PhytoComm	Yin Yang Huo	G098H1114821	62327	40	from supplier
PhytoComm	Yin Yang Huo	G098H1114821	62328	40	from supplier
PhytoComm	Yin Yang Huo	G098HS241SH1	62683	40	from supplier
PhytoComm	Yin Yang Huo	G098HS241SH1	62684	40	from supplier

Validation samples

A total of 37 534 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 *Yin Yang Huo*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Yin Yang Huo*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yin Yang Huo	G098H1114622	62221 [†]	20
PhytoComm	Yin Yang Huo	G098H1114622	62222 [†]	20
PhytoComm	Yin Yang Huo	G098H1114821	62327 [†]	20
PhytoComm	Yin Yang Huo	G098H1114821	62328 [†]	20
PhytoComm	Yin Yang Huo	G098HS241SH1	62683 [†]	20
PhytoComm	Yin Yang Huo	G098HS241SH1	62684 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Yin Yang Huo*.

Supplier	Substance	Batch	Spectra
Phytocomm	Yin Yang Huo	G098H1114422	2

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 849 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	1	240	0	23 960
Type B	0	118	2	12 362
Type C	0	0	2	849

The substance/substance group *Yin Yang 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	99.9962 % (> 99.9805 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	98.3333 % (> 95.8333 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62684	62684	0.00	3.51
62221	62221	0.00	11.44
62328	62328	0.00	13.06
62683	62683	0.00	3.71
62222	62222	0.00	10.68
62327	62327	0.00	12.91

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yu Jin**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60171-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Yu Jin; Curcumae tuber

Special notes

When selecting the *Yu Jin* substance/substance group, the following information is displayed to 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 Jin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yu Jin	G084HS357RN1	62277	40	from supplier
PhytoComm	Yu Jin	G084HS357RN1	62278	40	from supplier
PhytoComm	Yu Jin	G084H2201821	62517	40	from supplier
PhytoComm	Yu Jin	G084H2201821	62518	40	from supplier

Validation samples

A total of 37 534 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 *Yu Jin*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Yu Jin*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yu Jin	G084HS357RN1	62277 [†]	20
PhytoComm	Yu Jin	G084HS357RN1	62278 [†]	20
PhytoComm	Yu Jin	G084H2201821	62517 [†]	20
PhytoComm	Yu Jin	G084H2201821	62518 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Yu Jin*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Yu Jin* 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 Jin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 041
Type B	1	80	0	12 401
Type C	0	0	0	851

The substance/substance group *Yu Jin* 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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	99.9949 % (> 99.9645 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62277	62277	0.00	4.54
62517	62517	0.00	9.79
62278	62278	0.00	5.73
62518	62518	0.00	10.13

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yu Xing Cao**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60606-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Yu Xing Cao; Houlttuyniae 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	G124H1149823	62583	40	from supplier
PhytoComm	Yu Xing Cao	G124H1149823	62584	40	from supplier

Validation samples

A total of 37 534 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 *Yu Xing Cao*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Yu Xing Cao*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yu Xing Cao	G124H1149823	62583 [†]	20
PhytoComm	Yu Xing Cao	G124H1149823	62584 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Yu Xing Cao*.

Supplier	Substance	Batch	Spectra
Phytocomm	Yu Xing Cao	g124h1149122	1
Phytocomm	Yu Xing Cao	G124H1149222	1
Phytocomm	Yu Xing Cao	G124H1149423	2
Phytocomm	Yu Xing Cao	g124h1149222	1

- 846 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	40	0	12 442
Type C	0	0	5	846

The substance/substance group *Yu Xing 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8208 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62584	62584	0.00	11.69
62583	62583	0.00	12.12

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yu Zhu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60056-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Yu Zhu; Polygonati odorati rhizoma

Special notes

When selecting the *Yu 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 *Yu Zhu*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Yu Zhu	G195HS087SK1	62605	40	from supplier
PhytoComm	Yu Zhu	G195HS087SK1	62606	40	from supplier

Validation samples

A total of 37 534 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 *Yu Zhu*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Yu Zhu*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yu Zhu	G195HS087SK1	62605 [†]	20
PhytoComm	Yu Zhu	G195HS087SK1	62606 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Yu Zhu*.

Supplier	Substance	Batch	Spectra
Phytocomm	Yu Zhu	G195H0517421	2
PhytoComm	Yu Zhu	G195H0517121	1

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 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 *Yu 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	24 121
Type B	0	40	0	12 442
Type C	0	0	3	848

The substance/substance group *Yu Zhu* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62605	62605	0.00	8.53
62606	62606	0.00	8.43

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Yuan Zhi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60100-2019-09-24
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	G194HS306RP1	62431	40	from supplier
PhytoComm	Yuan Zhi	G194HS306RP1	62432	40	from supplier
PhytoComm	Yuan Zhi	G194HS306SH1	62557	40	from supplier
PhytoComm	Yuan Zhi	G194HS306SH1	62558	40	from supplier

Validation samples

A total of 37 534 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 *Yuan Zhi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Yuan Zhi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Yuan Zhi	G194HS306RP1	62431 [†]	20
PhytoComm	Yuan Zhi	G194HS306RP1	62432 [†]	20
PhytoComm	Yuan Zhi	G194HS306SH1	62557 [†]	20
PhytoComm	Yuan Zhi	G194HS306SH1	62558 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Yuan Zhi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Yuan Zhi	g194h140622	1
PhytoComm	Yuan Zhi	G194H1406222	1
Phytocomm	Yuan Zhi	G194H1406222	1
PhytoComm	Yuan Zhi	G194H1406522	1
Phytocomm	Yuan Zhi	G194H1406522	2

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	3	79	1	12 399
Type C	1	0	6	844

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	99.9848 % (> 99.9543 %)	98.7500 % (> 95.0000 %)
Type C	99.8843 % (> 99.2944 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62432	62432	0.00	5.03
62557	62557	0.00	5.26
62431	62431	0.00	4.67
62558	62558	0.00	5.69

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Ze Xie**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60165-2019-09-24
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	G011H1605821	62295	40	from supplier
PhytoComm	Ze Xie	G011H1605821	62296	40	from supplier
PhytoComm	Ze Xie	G011H1605822	62507	40	from supplier
PhytoComm	Ze Xie	G011H1605822	62508	40	from supplier

Validation samples

A total of 37 534 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 *Ze Xie*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Ze Xie*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Ze Xie	G011H1605821	62295 [†]	20
PhytoComm	Ze Xie	G011H1605821	62296 [†]	20
PhytoComm	Ze Xie	G011H1605822	62507 [†]	20
PhytoComm	Ze Xie	G011H1605822	62508 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 5 *Apo-Ident* customers from 4 batches from the substance/substance group *Ze Xie*.

Supplier	Substance	Batch	Spectra
Phytocomm	Ze Xie	g011h1605122	1
PhytoComm	Ze Xie	G011H1605122	1
Phytocomm	Ze Xie	G011H1605521	5
Phytocomm	Ze Xie	G011H1605422	1
PhytoComm	Ze Xie	G011H1605521	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 842 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	4	3	6	838

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.1898 % (> 98.5996 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62508	62508	0.00	6.03
62295	62295	0.00	12.61
62296	62296	0.00	12.90
62507	62507	0.00	6.54

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Zhe Bei Mu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50388-2019-09-24
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	G108H0712821	62339	40	from supplier
PhytoComm	Zhe Bei Mu	G108H0712821	62340	40	from supplier
PhytoComm	Zhe Bei Mu	G108HS138SG1	62687	40	from supplier
PhytoComm	Zhe Bei Mu	G108HS138SG1	62688	40	from supplier

Validation samples

A total of 37 534 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 *Zhe Bei Mu*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Zhe Bei Mu*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhe Bei Mu	G108H0712821	62339 [†]	20
PhytoComm	Zhe Bei Mu	G108H0712821	62340 [†]	20
PhytoComm	Zhe Bei Mu	G108HS138SG1	62687 [†]	20
PhytoComm	Zhe Bei Mu	G108HS138SG1	62688 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Zhe Bei Mu*.

Supplier	Substance	Batch	Spectra
PhytoComm	Zhe Bei Mu	G108H0712321	1
Phytocomm	Zhe Bei Mu	G108H0712422	1

- 849 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	1	80	0	12 401
Type C	0	0	2	849

The substance/substance group *Zhe Bei Mu* 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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	99.9974 % (> 99.9670 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62340	62340	0.00	22.20
62339	62339	0.00	22.41
62687	62687	0.00	8.89
62688	62688	0.00	8.82

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Zhi Ke**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60158-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Zhi Ke; Citri aurantii fructus

Special notes

When selecting the *Zhi Ke* substance/substance group, the following information is displayed to 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 Ke*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Zhi Ke	G043HS169RR1	62439	40	from supplier
PhytoComm	Zhi Ke	G043HS169RR1	62440	40	from supplier

Validation samples

A total of 37 534 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 Ke*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Zhi Ke*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhi Ke	G043HS169RR1	62439 [†]	20
PhytoComm	Zhi Ke	G043HS169RR1	62440 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 2 batches from the substance/substance group *Zhi Ke*.

Supplier	Substance	Batch	Spectra
Phytocomm	Zhi Ke	G043H0921221	1
Phytocomm	Zhi Ke	G043H0921422	2

- 848 spectra from 12 *Apo-Ident* customers from a total of 511 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Ke* 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 Ke* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 121
Type B	0	40	0	12 442
Type C	0	0	3	848

The substance/substance group *Zhi Ke* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8225 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62439	62439	0.00	9.19
62440	62440	0.00	9.16

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Zhi Mu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60196-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Zhi Mu; 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
PhytoComm	Zhi Mu	G019H0824821	62405	40	from supplier
PhytoComm	Zhi Mu	G019H0824821	62406	40	from supplier
PhytoComm	Zhi Mu	G019HS153SG1	62647	40	from supplier
PhytoComm	Zhi Mu	G019HS153SG1	62648	40	from supplier

Validation samples

A total of 37 534 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 *Zhi Mu*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 294 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group *Zhi Mu*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhi Mu	G019HS153QL1	62193 [†]	20
PhytoComm	Zhi Mu	G019HS153QL1	62194 [†]	20
PhytoComm	Zhi Mu	G019H0824821	62405 [†]	20
PhytoComm	Zhi Mu	G019H0824821	62406 [†]	20
PhytoComm	Zhi Mu	G019HS153SG1	62647 [†]	20
PhytoComm	Zhi Mu	G019HS153SG1	62648 [†]	20

- 12 362 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Zhi Mu*.

Supplier	Substance	Batch	Spectra
PhytoComm	Zhi Mu	G019H0824321	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 850 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	0	1	850

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8311 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well 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	14.78
62194	62194	0.00	13.86
62406	62406	0.00	11.98
62647	62647	0.00	8.71
62405	62405	0.00	11.69
62648	62648	0.00	9.26

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Zhi Shi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60145-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Zhi Shi; Aurantii fructus immaturus

Special notes

When selecting the *Zhi Shi* substance/substance group, the following information is displayed to 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 Shi*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
PhytoComm	Zhi Shi	G044H0922821	62389	40	from supplier
PhytoComm	Zhi Shi	G044H0922821	62390	40	from supplier
PhytoComm	Zhi Shi	G044HS168SK1	62655	40	from supplier
PhytoComm	Zhi Shi	G044HS168SK1	62656	40	from supplier

Validation samples

A total of 37 534 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 *Zhi Shi*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Zhi Shi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhi Shi	G044H0922821	62389 [†]	20
PhytoComm	Zhi Shi	G044H0922821	62390 [†]	20
PhytoComm	Zhi Shi	G044HS168SK1	62655 [†]	20
PhytoComm	Zhi Shi	G044HS168SK1	62656 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 14 spectra from 6 *Apo-Ident* customers from 5 batches from the substance/substance group *Zhi Shi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Zhi Shi	G044H0922221	2
Phytocomm	Zhi Shi	g044h0922221	1
PhytoComm	Zhi Shi	G044H0922321	2
Phytocomm	Zhi Shi	G044H0922321	2
PhytoComm	Zhi Shi	G044H0922221	3
phytocomm	Zhi Shi	g044h0922321	1
Phytocomm	Zhi Shi	G044H0922521	3

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 837 spectra from 12 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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 Shi* 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 Shi* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to 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	24 041
Type B	0	80	0	12 402
Type C	0	1	13	837

The substance/substance group *Zhi Shi* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8191 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62390	62390	0.00	20.97
62655	62655	0.00	12.36
62389	62389	0.00	20.90
62656	62656	0.00	11.61

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Zhi Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60367-2019-09-24
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	G110H1137822	62529	40	from supplier
PhytoComm	Zhi Zi	G110H1137822	62530	40	from supplier

Validation samples

A total of 37 534 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 Zi*. These samples are listed above in the [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Zhi Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhi Zi	G110H1137822	62529 [†]	20
PhytoComm	Zhi Zi	G110H1137822	62530 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Zhi Zi*.

Supplier	Substance	Batch	Spectra
Phytocomm	Zhi Zi	g110h1137121	1
PhytoComm	Zhi Zi	G110H1137121	1
Phytocomm	Zhi Zi	G110H1137521	3
PhytoComm	Zhi Zi	G110H1137521	1

- 845 spectra from 12 *Apo-Ident* customers from a total of 510 batches from a further 215 sub-

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

stances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	80	0	24 121
Type B	0	40	0	12 442
Type C	0	0	6	845

The substance/substance group *Zhi 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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8204 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62530	62530	0.00	14.92
62529	62529	0.00	14.85

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Zhu Ru**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60241-2019-09-24
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	G047HS109QM2	62207	40	from supplier
PhytoComm	Zhu Ru	G047HS109QM2	62208	40	from supplier
PhytoComm	Zhu Ru	G047HS109SK1	62657	40	from supplier
PhytoComm	Zhu Ru	G047HS109SK1	62658	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group *Zhu Ru*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zhu Ru	G047HS109QM2	62207 [†]	20
PhytoComm	Zhu Ru	G047HS109QM2	62208 [†]	20
PhytoComm	Zhu Ru	G047HS109SK1	62657 [†]	20
PhytoComm	Zhu Ru	G047HS109SK1	62658 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Zhu Ru*.

Supplier	Substance	Batch	Spectra
Phytocomm	Zhu Ru	G047H0625321	2
PhytoComm	Zhu Ru	G047H0625321	1
Phytocomm	Zhu Ru	g047h0625321	1
Phytocomm	Zhu Ru	G047h625321	1
phytocomm	Zhu Ru	g047h0625321	1
Phytocomm	Zhu Ru	G047H0625422	3

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 842 spectra from 12 *Apo-Ident* customers from a total of 509 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	10	144	16	24 031
Type B	10	60	20	12 392
Type C	0	0	9	842

The substance/substance group *Zhu Ru* 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	99.9657 % (> 99.9501 %)	90.0000 % (> 88.1250 %)
Type B	99.9289 % (> 99.8984 %)	75.0000 % (> 71.2500 %)
Type C	100.0000 % (> 98.8196 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62657	62657	0.00	3.40
62658	62658	0.00	3.44
62207	62207	0.00	2.54
62208	62208	0.00	2.75

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Zi Hua Di Ding**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50376-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Zi Hua Di Ding; Viola 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	G249HS269SK1	62627	40	from supplier
PhytoComm	Zi Hua Di Ding	G249HS269SK1	62628	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Zi Hua Di Ding*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zi Hua Di Ding	G249HS269SK1	62627 [†]	20
PhytoComm	Zi Hua Di Ding	G249HS269SK1	62628 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Zi Hua Di Ding*.

Supplier	Substance	Batch	Spectra
PhytoComm	Zi Hua Di Ding	G249H1216321	2

- 849 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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	1	80	0	24 120
Type B	0	39	1	12 442
Type C	0	0	2	849

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	99.9962 % (> 99.9806 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	97.5000 % (> 90.0000 %)
Type C	100.0000 % (> 98.8247 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62627	62627	0.00	6.75
62628	62628	0.00	4.74

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Zi Su Zi**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60133-2019-09-24
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	G183H1213822	62483	40	from supplier
PhytoComm	Zi Su Zi	G183H1213822	62484	40	from supplier

Validation samples

A total of 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Zi Su Zi*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zi Su Zi	G183H1213822	62483 [†]	20
PhytoComm	Zi Su Zi	G183H1213822	62484 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Zi Su Zi*.
- 851 spectra from 12 *Apo-Ident* customers from a total of 513 batches from a further 216 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

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	24 121
Type B	0	40	0	12 442
Type C	0	0	0	851

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.8182 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62483	62483	0.00	12.84
62484	62484	0.00	13.07

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **Zi Wan**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60155-2019-09-24
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 37 534 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 [calibration samples](#) section.
- 24 121 spectra from a total of 296 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Zi Wan*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	Zi Wan	G038H1215621	62045 [†]	20
PhytoComm	Zi Wan	G038H1215621	62046 [†]	20

- 12 442 spectra from a total of 298 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Zi Wan*.

Supplier	Substance	Batch	Spectra
Phytocomm	Zi Wan	G038H1215321	2

- 849 spectra from 12 *Apo-Ident* customers from a total of 512 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), 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*.

samples are listed in the *Type C* section of each substance page. If the substance 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	24 121
Type B	0	40	0	12 442
Type C	11	2	0	838

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 % (> 99.9689 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9394 %)	100.0000 % (> 85.0000 %)
Type C	98.9005 % (> 98.3128 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well 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	14.11
62046	62046	0.00	13.96

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group (Ku) Xing Ren
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 50290-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

(Ku) Xing Ren; Armeniaceae 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	G029H0708821	62393	40	from supplier
PhytoComm	(Ku) Xing Ren	G029H0708821	62394	40	from supplier
PhytoComm	(Ku) Xing Ren	G029H0708823	62509	40	from supplier
PhytoComm	(Ku) Xing Ren	G029H0708823	62510	40	from supplier

Validation samples

A total of 37 534 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 (Ku) Xing Ren. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group (Ku) Xing Ren.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	(Ku) Xing Ren	G029H0708821	62393 [†]	20
PhytoComm	(Ku) Xing Ren	G029H0708821	62394 [†]	20
PhytoComm	(Ku) Xing Ren	G029H0708823	62509 [†]	20
PhytoComm	(Ku) Xing Ren	G029H0708823	62510 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 10 spectra from 7 *Apo-Ident* customers from 6 batches from the substance/substance group (Ku) Xing Ren.

Supplier	Substance	Batch	Spectra
PhytoComm	(Ku) Xing Ren	G029H708125	1
Phytocomm	(Ku) Xing Ren	G029H0708125	2
PhytoComm	(Ku) Xing Ren	G029H0708125	1
Phytocomm	(Ku) Xing Ren	g029h0708122	1
PhytoComm	(Ku) Xing Ren	G029H0708322	2
phytocomm	(Ku) Xing Ren	g029h0708322	2
PhytoComm	(Ku) Xing Ren	G029H0708622	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 841 spectra from 12 *Apo-Ident* customers from a total of 507 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	0	0	10	841

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.8195 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62394	62394	0.00	54.03
62509	62509	0.00	60.73
62510	62510	0.00	60.88
62393	62393	0.00	53.05

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group (Sheng) Di Huang
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60005-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

(Sheng) Di Huang; Rehmanniae 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
PhytoComm	(Sheng) Di Huang	G211H0532822	62311	40	from supplier
PhytoComm	(Sheng) Di Huang	G211H0532822	62312	40	from supplier

Validation samples

A total of 37 534 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 (*Sheng*) *Di Huang*. These samples are listed above in the [calibration samples](#) section.
- 23 961 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 6 reference samples from the substance/substance group (*Sheng*) *Di Huang*.

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
PhytoComm	(Sheng) Di Huang	G211H0532822	62311 [†]	20
PhytoComm	(Sheng) Di Huang	G211H0532822	62312 [†]	20

- 12 362 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group (*Sheng*) *Di Huang*.

Supplier	Substance	Batch	Spectra
Phytocomm	(Sheng) Di Huang	g211h053221	1

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[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

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Supplier	Substance	Batch	Spectra
Phytocomm	(Sheng) Di Huang	g211h0532121	1
	(Sheng) Di Huang	g211h0532323	1
Phytocomm	(Sheng) Di Huang	G211H0532521	4
PhytoComm	(Sheng) Di Huang	G211H0532621	1

- 843 spectra from 12 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	240	0	23 961
Type B	0	120	0	12 362
Type C	0	1	7	843

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 % (> 99.9687 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.8198 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well 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	11.87

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62311	62311	0.00	9.86
61881	61881	0.00	15.03
61804	61804	0.00	13.16
62312	62312	0.00	10.19
61882	61882	0.00	14.89

VALIDATION REPORT

IdentModul 2.0-2019-04

Validated substance/substance group **(Shi) Chang Pu**
Substance class TCM - Granulated herbal extracts (PhytoComm)
Report date 24/09/2019
Report number 60426-2019-09-24
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

(Shi) Chang Pu; 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
PhytoComm	(Shi) Chang Pu	G006H0544821	62399	40	from supplier
PhytoComm	(Shi) Chang Pu	G006H0544821	62400	40	from supplier

Validation samples

A total of 37 534 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 (*Shi*) *Chang Pu*. These samples are listed above in the [calibration samples](#) section.
- 24 041 spectra from a total of 295 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 4 reference samples from the substance/substance group (*Shi*) *Chang Pu*.

Supplier	Substance	Batch	Sample ID	Spectra
PhytoComm	(Shi) Chang Pu	G006H0544622	62107 [†]	20
PhytoComm	(Shi) Chang Pu	G006H0544622	62108 [†]	20
PhytoComm	(Shi) Chang Pu	G006H0544821	62399 [†]	20
PhytoComm	(Shi) Chang Pu	G006H0544821	62400 [†]	20

- 12 402 spectra from a total of 297 batches from further 163 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 3 *Apo-Ident* customers from 5 batches from the substance/substance group (*Shi*) *Chang Pu*.

Supplier	Substance	Batch	Spectra
Phytocomm	(Shi) Chang Pu	G006H0544122	1
Phytocomm	(Shi) Chang Pu	G006H0544322	1
Phytocomm	(Shi) Chang Pu	G006HS2700N1	1
Herbasinica	(Shi) Chang Pu	g006h0544321	1
Phytocomm	(Shi) Chang Pu	g006h0544023	1

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 846 spectra from 12 *Apo-Ident* customers from a total of 508 batches from a further 215 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance 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	160	0	24 041
Type B	0	80	0	12 402
Type C	4	1	4	842

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 % (> 99.9687 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9391 %)	100.0000 % (> 92.5000 %)
Type C	99.3981 % (> 98.8085 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
62400	62400	0.00	8.22
62399	62399	0.00	9.02
62107	62107	0.00	12.00
62108	62108	0.00	12.02

Appendix A: Additional calibration samples (Type A)

Not required.

Appendix B: Additional validation samples (Type B)

Not required.

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 129 batches. From these, 183 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	1
Mediherb	Zhu Ling		1
phytocomm	Ce Bai Ye	g050h0975321	2
phytocomm	Chan Tui	g067h1817322	1
phytocomm	Di Long	g148h603321	1
phytocomm	Lu Jiao Jiao	G323H1158321	1
phytocomm	Niu Bang Zi	g026h0433321	2
Phytocomm	(Bai) Dou Kou	G016H0508521	1
Phytocomm	(Bai) Dou Kou	G016H0508521	1
Phytocomm	(Bai) Jiang Can	G269H0513321	2
Phytocomm	(Bai) Jiang Can	g269h0513222	1
Phytocomm	(Bai) Jiang Can	g144h1708221	1
Phytocomm	(Huai) Niu Xi	G003H1905422	2
Phytocomm	(Huai) Niu Xi	G003H1905222	2
Phytocomm	(Huai) Niu Xi	g003h1905222	1
Phytocomm	(Huai) Niu Xi	G003H1905321	3
Phytocomm	Ai Ye	G033H0613022	1
Phytocomm	Ai Ye	G033H0613421	1
Phytocomm	Bai Bu	G235H0608321	1
Phytocomm	Bai Guo	G114H0509521	1
Phytocomm	Bai Guo	G114H0509321	2
Phytocomm	Bai Jiang Cao	G181H1180422	1
Phytocomm	Bai Jiang Cao	G181H1180321	1
Phytocomm	Bai Tou Weng	G207H0511521	4
Phytocomm	Bai Zhi	G020H0503421	1
Phytocomm	Ban Lan Gen	G128H0816421	2
Phytocomm	Bo He	g158h1712022	1
Phytocomm	Ce Bai Ye	G050H0975321	1
Phytocomm	Ce Bai Ye	G050HS245	1
Phytocomm	Chan Tui	G067H1817323	2
Phytocomm	Chan Tui	G067H1817322	3
Phytocomm	Chong Wei Zi	g317bp021046	1
Phytocomm	Chuan Bei Mu	G107BP020722A	1
Phytocomm	Chuan Bei Mu	g107f110721	2
Phytocomm	Chuan Mu Tong	G009H0310321	1
Phytocomm	Chuan Mu Tong	g009h0310321	1
Phytocomm	Chuan Niu Xi	g318h0431321	1
Phytocomm	Da Fu Pi	G293H0321221	1
Phytocomm	Da Qing Ye	G127H0318421	2
Phytocomm	Deng Xin Cao	f100707	1
Phytocomm	Di Fu Zi	G131H0605122	1
Phytocomm	Di Long	G148H0603321	2
Phytocomm	Di Long	G148H0603421	2
Phytocomm	Di Yu	G215H0604322	2
Phytocomm	Ding Xiang	G058H0210021	1
Phytocomm	E Jiao	G036H0861421	2

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Supplier	Substance	Batch	Spectra
Phytocomm	E Jiao	g036h0861221	1
Phytocomm	E Jiao	g036h0861121	1
Phytocomm	Fu Pen Zi	g213h1813122	1
Phytocomm	Gu Sui Bu	g094h1011023	1
Phytocomm	Gu Sui Bu	g094h1011221	1
Phytocomm	Gu Sui Bu	G094H1011221	3
Phytocomm	Gua Lou Ren	g243h1095123	1
Phytocomm	Huai Hua	G263H1423421	1
Phytocomm	Ji Nei Jin	G259H2102321	1
Phytocomm	Ji Nei Jin	g259h2102321	1
Phytocomm	Jie Cao	H2111921	1
Phytocomm	Jue Ming Zi	G059H1097221	3
Phytocomm	Lu Jiao Shuang	FB1419901	1
Phytocomm	Lu Jiao Shuang	G062H1419421	1
Phytocomm	Lu Lu Tong	G142H1336521	2
Phytocomm	Lu Lu Tong	G142H1336321	1
Phytocomm	Mi Huan Jun	G510H0418422	1
Phytocomm	Mi Huan Jun	G510H0418221	1
Phytocomm	Mu Zei	G265H0427421	1
Phytocomm	Niu Bang Zi	G026H0433521	3
Phytocomm	Niu Bang Zi	G026H0433321	3
Phytocomm	Qian Hu	G185H0926322	4
Phytocomm	Qian Shi	G102H0836422	1
Phytocomm	Quan Xie	G222F110314	1
Phytocomm	Ren Shen	g115ho562121	1
Phytocomm	Sang Piao Xiao	G282H421029201	1
Phytocomm	Sang Shen	G163H1047221	2
Phytocomm	Sang Shen	G163H1047121	1
Phytocomm	Shan Zha	G082H0331324	1
Phytocomm	Shan Zha	G082H0331521	1
Phytocomm	She Chuang Zi	G076H1154122	1
Phytocomm	Wu Gong	G311H1411321	1
Phytocomm	Wu Gong	G311H411321	1
Phytocomm	Wu Jia Pi	g002h0402321	1
Phytocomm	Wu Zhu Yu	G103H0766022	1
Phytocomm	Xian Mao	G304H0549521	2
Phytocomm	Xian Mao	G304H0549321	2
Phytocomm	Xiao Hui Xiang	g104h0339321	1
Phytocomm	Xiao Hui Xiang	G104H0339522	3
Phytocomm	Xuan Fu Hua	G126H1168521	1
Phytocomm	Ze Lan	G268H1606421	1
Phytocomm	Ze Lan	g268h1606221	1
Phytocomm	Zhen Zhu Mu	g155h0979221	1
Phytocomm	Zhi Gan Cao	G118H0881522	4
Phytocomm	Zhi Gan Cao	g118h0881322	1
Phytocomm	Zhu Ling	G199H1509421	2
PhytoComm	(Bai) Jiang Can	G269H0513222	1
PhytoComm	(Fen) Bi Xie	G0290H1251121	1
PhytoComm	(Huai) Niu Xi	G003H190522	1
PhytoComm	Ai Ye	G033H0613021	1
PhytoComm	Bai Bu	G235H0608221	1
PhytoComm	Bai Tou Weng	G207H0511221	3
PhytoComm	Bie Jia	G507H2401321	1
PhytoComm	Bie Jia	G507H2401121	1
PhytoComm	Bo He	G158H1712121	1
PhytoComm	Cao Guo	E241050	1
PhytoComm	Chuan Bei Mu	G107F110721	1
PhytoComm	Chuan Mu Tong	G009H0310521	1
PhytoComm	Chuan Niu Xi	G318H0431321	1
PhytoComm	Di Long	G148H0603022	1

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Supplier	Substance	Batch	Spectra
PhytoComm	E Bu Shi Cao	G061H180122	1
PhytoComm	E Jiao	G036H0861221	4
PhytoComm	Geng Mi	G329H1320121	1
PhytoComm	Gu Sui Bu	G094H1011522	1
PhytoComm	Gua Lou Ren	G243H1095421	1
PhytoComm	He Zi	G291H1239221	2
PhytoComm	Jue Ming Zi	G059H1097221	1
PhytoComm	Kuan Dong Hua	H1219921	1
PhytoComm	Long Gu	G025H1706122	1
PhytoComm	Lu Lu Tong	G142H1336122	1
PhytoComm	Ma Chi Xian	G255F110310	1
PhytoComm	Mu Zei	G265H0427823	1
PhytoComm	Qian Shi	G102H0836121	1
PhytoComm	She Chuang Zi	G076H1154021	1
PhytoComm	Suo Yang	G260H1831121	1
PhytoComm	Wu Jia Pi	G002H0402321	4
PhytoComm	Wu Zhu Yu	G103H0766321	1
PhytoComm	Ze Lan	G268H1606221	2
PhytoComm	Zhi Gan Cao	G118H0881322	1
PhytoComm	Zhu Ling	G199H1509521	1
PhytoComm	Zhu Ling	G199H1509022	1
PhytoComm	Zi Su Ye	G182H1214321	3
PhytoComm	Zi Su Ye	G182HS2680P1	1

Appendix D: Requirements of validation

In order to ensure adherence to the safe scientific status, the individual methods for manufacturing and testing must be validated under certain circumstances (compare § 34 para. 1 no. 3, § 35 para. 1 no. 4 and para. 4 sentence 1 no. 2 b, para. 6 sentence 3 *ApoBetrO* [Pharmacies Rules and Regulations]). The *ApoBetrO* [Pharmacies Rules and Regulations] incorporates a legal definition in § 1 a para. 16 (quotation translated):

“Validation is the provision of documented proof which with a high degree of safety documents that, via a specific process or standard work process, a medicinal product is manufactured and tested, which is in accordance with previously determined quality features.”

Validation documentation can be used to prove that methods or devices which are not described in the Pharmacopoeia within the meaning of § 6 para. 1 sentence 3 *ApBetrO* [Pharmacies Rules and Regulations] achieve the same results as those in the Pharmacopoeia. On the other hand, with the requirements of the demanded validation it must be observed whether the respective testing method is already incorporated in the Pharmacopoeia.

NIR spectroscopy as a general testing method need not be validated in accordance with the express ruling in the *Ph. Eur. Section 1.1* [3], as it is already described in *Section 2.2.40* of the *Ph. Eur.* as an area of application for the identification of raw materials.

However, a special validation requirement exists for the reference database. This requirement is met with the existing document. Further requirements or rules as to how this proof must be furnished do not exist. It is required that the processes guarantee the same results as the methods and devices in the Pharmacopoeia [17].

Carrying out identity tests with *Apo-Ident* is therefore also possible if the NIR spectroscopy process is not required in the Pharmacopoeia monograph of the substance for identity testing. All NIR analyses with *Apo-Ident* prove several, often all molecule groups and are therefore comparable with a series of individual, targeted chemical proofs [4]. Therefore, the identity proof with *Apo-Ident* replaces the monograph test series (with two or more test combinations).

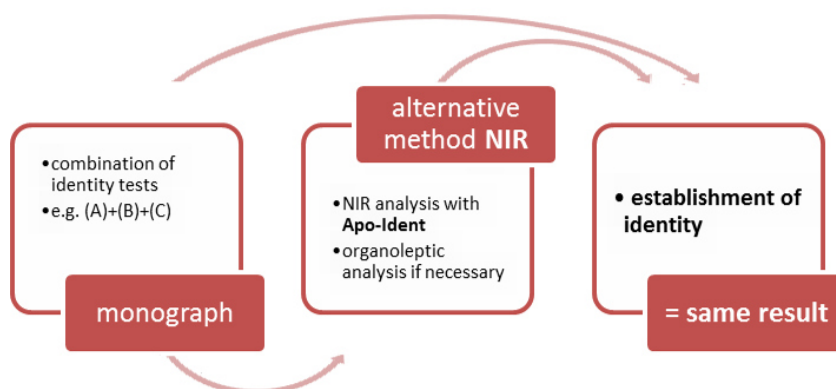


Figure 2: The combination of tests of the monograph is replaced by the alternative method NIR spectroscopy using *Apo-Ident*. This is permissible because both test procedures result in the establishment of the identity of the raw material.

With this validation documentation, proof is furnished that identical results are achieved with *Apo-Ident* and Pharmacopoeia methods, i.e. confirmation of the identity of the raw material [2].

Appendix E: Conformity of Apo-Ident with the European pharmacopeia

According to *Ph. Eur. Section 2.2.40*, NIR spectroscopy is basically suitable for: “Identification of agents, excipients, dosage forms, intermediate manufacturing products, chemical raw materials and packaging materials” ([3], quotation translated).

The fact that *Apo-Ident* meets the further criteria of the European Pharmacopoeia under the headings in *Section 2.2.40*

- Apparatus
- Measurement methods
- Sample preparation and presentation
- Testing the functionality of the instrument
- Identification and characterisation (qualitative analysis)
- Quantitative analysis
- Ongoing model evaluation
- Transfer of databases
- Data storage

can be proven based on the *HiperScan GmbH* documentation of “Meeting 2.2.40 *Ph. Eur.* by *Apo-Ident*” [4].

Appendix F: Addition to the second-stage models

As described in the general part of the *Apo-Ident* validation documentation, in the section [Model creation procedure and validation runs](#), under 2. *Generating the chemometric models (calibration) in f)*, it is possible to create a further chemometric model for certain substances (second-stage model) and to undertake the assessment in several steps.

Substances in second-stage models

In the *Apo-Ident Update 2019-04*, a distinction is made between the following substances in the listed second-stage models:

Submodel 1

Bacitracin
Betamethasone, micronized
Betamethasone valerate
Budesonide, micronized
Capsaicin
Dexamethasone
Erythromycin
Heparin sodium
Norethisterone acetate
Prednicarbate, micronized
Prednisolone, micronized
Prednisone
Triamcinolone, micronized
Triamcinolone acetonide

Submodel 2

Beclometasone dipropionate, anhydrous
Betamethasone dipropionate, micronized
Clobetasol propionate
Diphenylcyclopropenone
Gentamicin sulfate
Sodium benzoate
Sodium citrate
Oxybutynin hydrochloride

Submodel 3

Alfatradiol
Estriol
Pregnenolone
Progesterone, micronized
Quinine hydrochloride
Quinine sulfate dihydrate
Spironolactone
Testosterone propionate

Liquid submodel

2-ethylhexyl laurate
Base cream DAC

Eucerin® cum Aqua
Lanette® ointment (conserved)
Non-ionic hydrophil ointment
Squalane
Wool alcohols cream DAB
Wool alcohols cream SR

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